Universidade de Aveiro Departamento de Matemática
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Dissertação apresentada à Universidade de Aveiro para cumprimento dos requisitos necessários à obtenção do grau de Doutor em Matemática, realizada sob a orientação científica de Paula Cristina Supardo Machado Marques Cerejeiras, Professora Associada do Departamento de Matemática da Universidade de Aveiro.

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Dedico este trabalho à minha Esposa, aos meus Pais e ao meu Irmão por todo o apoio e compreensão ao longo destes quatro anos de trabalho.

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palavras-chave

Análise de Clifford, bases de Witt, teoria hipoeliptica, operador de Dirac parabólico, operadors não estacionários, decomposição de Fischer, processo de regularização, decomposição do espaço L_p, diferenças finitas, soluções fundamentais discreta e contínua, equação de Schrödinger não-linear cúbica.

resumo

Inicialmente, mostraremos que é possível resolver o problema de Schrödinger usando a teoria de semigrupos e a teoria hipoeliptica. No entanto, vamos verificar que as conclusões obtidas através destas abordagens não são as melhores quando se pretende fazer uma implementação numérica dos resultados teóricos.

Assim, de modo a ultrapassar os problemas de implementação usaremos a análise de Clifford para apresentar uma factorização para operadores do tipo $-\Delta \pm \alpha\partial_t$ usando a extensão do operador de Dirac parabólico $D_{\pm} = D + f\partial_t \pm \alpha f^{+}$.

No caso do operador de calor ($\alpha = 1$), é possível construir uma decomposição de Fischer. Esta decomposição pode ser aplicada na caracterização das potências do operador homogéneo associado a $D_{\pm}$.

Para o caso do operador de Schrödinger ($\alpha = i$), vamos aplicar um processo de regularização de modo a controlar a singularidade não removível existente no hiperplano *t=0*. Irão ser obtidos os operadores integrais regularizados que estão associados a este operador diferencial, nomeadamente, os operadores de Teodorescu e Cauchy-Bitsadze. O estudo das propriedades destes operadores integrais permitirá obter uma decomposição do espaço L_p, em termos do núcleo do operador de Dirac parabólico, para o caso regularizado e para o caso geral.

No último capítulo mostraremos que é possível estudar o problema de Schrödinger não-linear cúbico, utilizando uma combinação entre bases de Witt e diferenças finitas. Mostraremos também que é possível construir uma solução fundamental discreta, para os casos implícito e explícito do operador de Schrödinger discreto, usando o símbolo do operador de Laplace via transformada de Fourier. Em ambos os casos podemos provar a convergência das soluções fundamentais discretas obtidas para a correspondente contínua segundo a norma l_1. Com as conclusões anteriores, podemos apresentar um esquema numérico convergente e estável para o problema de Schrödinger não-linear cúbico.

keywords

Clifford analysis, Witt basis, hypoelliptic theory, parabolic Dirac operator, time dependent operators, Fischer decomposition, regularization procedure, L_p- decomposition, finite difference approximations, discrete and continuous fundamental solutions, cubic Schrödinger equation.

abstract

Initially, we will show that it is possible to solve the Schrödinger problem using the semigroup and hypoelliptic theories. However, we will see that the obtained conclusions are not the most appropriate for numerical implementations.

Therefore, in order to overcome this problem, we will use Clifford analysis to present a factorization for the operators $-\Delta \pm \alpha\partial_t$ using the parabolic-type Dirac operator $D_{\pm} = D + f\partial_t \pm \alpha f^+$.

In the case of the heat operator ($\alpha = 1$) we show that it is possible to construct a Fischer decomposition. This decomposition can be applied in the characterization of the powers of the homogeneous operator associated to $D_{\pm}$.

For the case of the Schrödinger operator ($\alpha = i$), we will apply a regularization procedure in order to control the non-removable singularity existing in the hyperplane *t=0*. We will study the arising operators such as the regularized Teodorescu and Cauchy-Bitsadze operators. The properties of these operators will be use to obtain a decomposition of the L_p space for the regularized case and general case, in terms of the kernel of the parabolic Dirac operator D_-.

In the last chapter of this thesis we show that it is possible to study the cubic non-linear Schrödinger problem using a combination of Witt basis and finite difference approximations. We will show that it is possible to construct a discrete fundamental solution for the explicit and implicit time dependent discrete Schrödinger operator, via discrete Fourier transform and the arising symbol of the Laplace operator. In both cases, we can prove the convergence of the obtained discrete fundamental solutions to the continuous one in l_1 norm. With the previous conclusions we can present a convergent and stable numerical scheme for solving the cubic non-linear Schrödinger problem.

Contents

List of Figures

List of Tables

Introduction

"It will be interest mathematical circles that the mathematical instruments created by the higher algebra play an essential part in the rational formulation of the new quantum mechanics."

Niels Bohr

In the begin of the XX century, the scientific community had realized that classical mechanics were not adequate to describe microscopic effects. In 1926, Erwin Schrödinger proposed his celebrated equation

$$H(x)\psi(x,t) = \pm i\hbar\partial_t\psi(x,t),$$

where i is the imaginary unit, x is space-variable, t is time-variable, ∂_t is the partial derivative with respect to t, $\hbar$ is the reduced Planck's constant (Planck's constant divided by 2π), $\psi(x,t)$ is the wave function, $H(x)$ is the Hamiltonian (self-adjoint operator acting on the space variable), and $\pm$ represents the forward/backward case, respectively, which soon became a corner stone in the new emergent field of quantum mechanics. Quantum mechanics are the laws which model microscopic system and interactions within, where atoms behave both as a wave and as a particles. A quantum state (wave-function or state-vector) describes a particle position inside a given system. Hence, the importance of the basic Schrödinger equation which describes the changes in time of the quantum state of a hydrogen atom. Based on this, several other phenomena are modeled. For example, the non-linear Schrödinger equation (NLS) provides a canonical description for the envelope dynamics of quasi-monochromatic plane wave (the carrying wave) propagating in a weakly non-linear dispersive medium when dissipative processes are negligible. On short times and small propagation distances, the dynamics are linear, but cumulative non-linear interactions result in a significant modulation of the wave amplitude on large spatial and temporal scales. The NLS equation expresses how the linear dispersion relation is affected by the thickening of spectral lines associated to the modulation and the resonant non-linear interactions.

One important feature in the Schrödinger equation is the fact that it is an instationary equation and, therefore, one cannot use standard elliptic theory for its resolution. Besides requiring special techniques for its treatment it is also subject to blow-up effects, which represents an additional problem. In this thesis we present some resolution methods for it based on Clifford algebras.

Clifford algebras were discovered by W.K. Clifford in 1878 as a generalization of the algebra of quaternions of W. R. Hamilton. Following a period of little activity, Clifford algebras were retaken in the $1930'$s as alternative approaches to vector calculus in Euclidean and non-Euclidean spaces in connection with the theory of electron spin (for example, see [40]).

Many of the classical problems of physics and their associated equations can be simplified by using such algebras, and this due to its intrinsic geometric nature. Dirac's solution to the relativistic electron equation becomes in this setting the solution of a simple first order PDE (see [23]). Same can be said of the solution by Onsager [53] of the two-dimensional Ising model, or of the study of the Maxwell's equations (see [56], [40], [45], [59]). Clifford algebras are routinely used to compute particle scattering cross-sections, and form the basic tool of quantum electrodynamics. Research in space-time symmetries, unification theory, and super-symmetry are looking at Clifford algebras for appropriate models (see, for example, [12], [24]).

In this thesis we use the relation between the Dirac and the heat equation introduced in [19]. We recall here that the heat equation is one standard model for parabolic equations.

Compared to the heat operator, the Schrödinger one presents an additional difficulty since its fundamental solution possesses (non-removable) singularities in the hyperplane $t = 0$. To overcome this problem, we resort to a standard regularization procedure (see [64], [66] for details) which allows some degree of control over these singularities and, thus, enables the application of the well-known theory of hypoelliptic boundary-value problems when constant coefficients are involved. Below we highlight the three main techniques used in this work.

Hypoelliptic theory was initiated by Hörmander in [43], where a necessary and sufficient condition for a solution of a homogeneous boundary-value problem to be C^∞ up to boundary of the domain was given. His condition, of an algebraic nature, was formulated in terms of behaviour near the infinity of the zeros of the so called characteristic function of the boundary-value problem. Roughly speaking, Hörmander's condition is similar to the algebraic condition that characterizes hypoelliptic partial differential operators with constant coefficients. For a brief summary of the basic notions and results on hypoelliptic we refer to Appendix A.

For this kind of operators we have existence techniques, for instance, see [28]. In there, the authors constructed explicitly the kernel of the heat operator in terms of a convenient perturbation of the semigroup associated to the Laplacian, thus providing a method for studying time-evolution equations. Connections between semigroup theory and the Schrödinger equation was already developed by many authors, for example, in [70], where the author constructed the semigroup operator associated via the infinitesimal generator. This approach didn't use any type of regularization procedure, hence, the construction of the semigroup was neither direct or immediate.

Barros-Neto [6] gave another characterization of the same problem based on regularity properties of the fundamental kernels associated to the boundary-value problem under consideration. With the help of such kernels, parametrices of the boundary-value problem can be constructed which in turns allows to obtain an explicit solution for the problem, although it is a rather complicated method to implement.

Finally, potential theory also provides a tool to solve boundary value problems via integral equations involving the fundamental solutions of the involved operators. This will allow us the implementation of the theory developed by K. Gürlebeck and W. Sprößig which is based on orthogonal decomposition of the underlying function space where one of the subspaces is the space of null-solutions of the corresponding Dirac operator. Again, a regularization procedure is necessary.

Hence, the structure of this thesis is the following one: in Chapter 1 we present some preliminaries concepts concerning Clifford algebras, the functional spaces and respective norms necessary, we recall some basics from tensorial calculus and vector bundles. We finish this chapter we a short resume of the study of the Laplace equation.

In Chapter 2 we combine semigroup and hypoelliptic theories in order to solve the linear Schrödinger problem. Also, we present an additional treatment for the case when the Laplace operator is replaced by the Bochner-Laplacian or by the Günter-Laplacian, in which cases the operator then takes into account the geometry of the underlined manifold.

Chapter 3 is divided in two topics: first, we present a factorization for the operators $-\Delta \pm \alpha\partial_t$ done by means a parabolic-type Dirac operator, i.e., an operator of the form $D_\pm = D + \mathfrak{f}\partial_t \pm \alpha\mathfrak{f}^\dagger$ such that $D_\pm^2 = -\Delta \pm \alpha\partial_t$. We give a characterization for the homogeneous operators associated to each of $D_\pm$ and we study the corresponding Fischer decomposition and associated powers of such homogeneous operator.

On a second part, we apply this factorization to the regularized sequence of operators associated to the Schrödinger operator $-\Delta + i\partial_t$. This enable us to successfully obtain correspondent sequences of regularized Teodorescu and Cauchy-Bitsadze operators. Their main properties are proven and used in order to derive a L_p-decomposition of the space of solutions of the Schrödinger equation.

In the last chapter, our aim is to study the numerical solution of (modified version of) the cubic non-linear Schrödinger (cubic NLS) problem using an appropriated combination of Witt basis and finite difference approximations. For that propose we construct a discrete fundamental solution for the explicit and implicit time dependent Schrödinger operator. This construction is done via a discrete Fourier transform and the arising symbol for the Laplace operator (see [37]). We prove the convergence of the discrete fundamental solutions to the continuous ones in the l_1 norm. With these conclusions we prove the convergence of a numerical scheme for solving the cubic NLS problem. We end this chapter with some numerical examples.

"The views of space and which I wish to lay before you sprung from the soil of experimental physics, and therein lies their strength. They are radical. Henceforth space by itself, and time by itself, are doomed to fade away into mere shadows, and only a kind of union or the two will preserve an independent reality"

Hermann Minkowski

Chapter 1

Preliminaries

"At the moment I am struggling with a new atomic theory.

If only I knew more mathematics!"

Erwin Schrödinger

1.1 Clifford Algebras

One of the main reasons for the success of complex analysis is that it allows to combine geometrical ideas with relatively simple analytic concepts. In this section we introduce Clifford algebras, which allow similar constructions in higher dimensions. Unfortunately, these algebras do not carry trough all properties - for instance, commutativity is lost. On the other hand, Clifford algebras allow an analytic manipulation of several geometrical entities such as $k-$blades view here as oriented $k-$volumes. Shortly speaking, a Clifford algebra is constructed from a finite-dimensional vector space with a scalar product by introducing an algebra multiplication which reflects both the properties of the existent scalar product and of the classic outer product in $\mathbb{R}^3$.

1.1.1 Real Clifford algebras

In this section we follow the notations and conventions established in [22]. Further details and approaches can be found in [11], [34], [39].

Basic definitions

Consider the pair $(\mathbb{R}^n, \mathcal{B})$, with $\mathcal{B}$ a real non-degenerate symmetric bilinear form on $\mathbb{R}^n$, i.e., a bilinear form $\mathcal{B} : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ which verifies:

(i) *Bilinearity condition*: For all $\lambda \in \mathbb{R}$, and for all $v, v', w, w' \in \mathbb{R}^n$

$$\mathcal{B}(\lambda v + v', w) = \lambda \mathcal{B}(v, w) + \mathcal{B}(v', w)$$
$$\mathcal{B}(v, \lambda w + w') = \lambda \mathcal{B}(v, w) + \mathcal{B}(v, w')$$

(ii) *Symmetry condition*: For all $v, w \in \mathbb{R}^n$

$$\mathcal{B}(v, w) = \mathcal{B}(w, v).$$

(iii) *Non-degeneracy condition* For each non-zero vector $v \in \mathbb{R}^n$ there exists a $w \in \mathbb{R}^n$ such that $\mathcal{B}(v, w) \neq 0$.

In these conditions, we say that the pair $(\mathbb{R}^n, \mathcal{B})$ is a non-degenerate real orthogonal space. By associating a matrix M to the bilinear form $\mathcal{B}$ with respect to a given basis of $\mathbb{R}^n$, we obtain a symmetric and non-singular matrix. Therefore, it will exists an orthonormal basis $e = \{e_1, ..., e_n\}$ of $\mathbb{R}^n$ for which

(1) $\mathcal{B}(e_i, e_i) = \begin{cases} 1 & , \quad i = 1, ..., p \\ -1 & , \quad i = p+1, ..., p+q \end{cases}$,

(2) $\mathcal{B}(e_i, e_j) = 0$, $i \neq j$,

for an unique pair (p, q), with $p + q = n$ (the uniqueness of this pair is derived from Sylvester's theorem). We will say then that $(\mathbb{R}^n, \mathcal{B})$ is a non-degenerate real orthogonal space of type (p, q) and we write $(\mathbb{R}^n, \mathcal{B}) = \mathbb{R}^{p,q}$.

Based on this pair, we define a real-valued Clifford algebra as:

Definition 1.1.1 *Let $\mathbb{R}^{p,q}, p + q = n$, be a non-degenerate real orthogonal space and let $\mathcal{A}$ be a real associative algebra with identity such that*

(i) $\mathcal{A}$ contains copies of $\mathbb{R}$ and $\mathcal{A}$ as linear subspaces.

(ii) For all $v \in \mathbb{R}^n$, $v^2 = \mathcal{B}(v, v)$.

(iii) $\mathcal{A}$ is generated, as a real algebra, by $\{1\}$ and $\mathbb{R}^n$.

Then $\mathcal{A}$ is said to be a real Clifford algebra associated to $\mathbb{R}^{p,q}$.

Moreover, for an orthonormal basis $e = \{e_1, ..., e_n\}$ of $\mathbb{R}^{p,q}$ the requirement (ii) of the previous definition implies

$$e_i^2 = \mathcal{B}(e_i, e_i) = \begin{cases} 1 & , \quad i = 1, ..., p \\ -1 & , \quad i = p+1, ..., p+q \end{cases} \tag{1.1}$$

and

$$e_i e_j + e_j e_i = 0, \qquad i \neq j, \tag{1.2}$$

in the algebra.

Indeed, (1.1) follows directly from the condition (ii) of the previous definition, while (1.2) is obtained by observing that for all $i \neq j$, on the one hand

$$\begin{aligned} (e_i + e_j)^2 &= \mathcal{B}(e_i + e_j, e_i + e_j) \\ &= \mathcal{B}(e_i, e_i) + \mathcal{B}(e_j, e_j) \\ &= e_i^2 + e_j^2, \end{aligned}$$

while on the other hand

$$(e_i + e_j)^2 = e_i^2 + e_j^2 + e_i e_j + e_j e_i.$$

A basis for the Clifford algebra $\mathcal{A}$

Let $\mathcal{A}$ be a Clifford algebra associated to $\mathbb{R}^{p,q}$ and let $e = \{e_1, ..., e_p, e_{p+1}, ..., e_{p+q}\}$ be an orthonormal basis for $\mathbb{R}^{p,q}$ $(p+q = n)$. Then, it follows from (1.1) that among all the products of two basis vectors e_i and e_j, it suffices to consider those products $e_i e_j$ for which $i < j$.

For each subset $A = \{\alpha_1, \ldots, \alpha_h\}$ of $N = \{1, \ldots, n\}$, with $1 \leq \alpha_1 < \alpha_2 < \ldots < \alpha_h \leq n$, we define $e_A = e_{\alpha_1} e_{\alpha_2} \cdots e_{\alpha_h}$ and $e_\emptyset = 1$. Then the preceding observations imply that the family

$$(e_\emptyset,\ e_A :\ A = \{\alpha_1, ..., \alpha_h\},\ 1 \leq \alpha_1 < \alpha_2 < ... < \alpha_h \leq n) \tag{1.3}$$

generates $\mathcal{A}$. Hence, $\dim(\mathcal{A}) \leq 2^n$.

We say that $\mathcal{A}$ is a real universal Clifford algebra whenever $\dim(\mathcal{A}) = 2^n$, and we denote it then as $\mathcal{A} = \mathbb{R}_{p,q}$. Moreover, we have for an arbitrary element $x \in \mathbb{R}_{p,q}$ that

$$x = \sum_{A \subset N} x_A e_A,$$

with $x_A \in \mathbb{R}$. In particular, $x \in \mathbb{R}^{p,q}$ implies $x = \sum_{j=1}^{n} x_j e_j$.

Now, we define the conjugation as an involution in the real universal Clifford algebra $\mathbb{R}_{p,q}$ given by its action on the basis vectors

$$\overline{e}_i = -e_i, \qquad i = 1, \cdots, n, \qquad \overline{1} = 1,$$

and which satisfies the following properties

$$\overline{\lambda x + y} = \lambda \overline{x} + \overline{y} \qquad\qquad \overline{(xy)} = (\overline{y})(\overline{x}) \qquad\qquad \overline{\overline{x}} = x,$$

for $x, y \in \mathbb{R}_{p,q}$ and $\lambda \in \mathbb{R}$.

1.1.2 Complex Clifford algebra

For future treatment of the Schrödinger equation, we need to define complex Clifford algebras. We will construct a complex Clifford algebra by means of (real) tensor product between the real universal Clifford algebra $\mathbb{R}_{p,q}$ and the complex field $\mathbb{C}$, that is

$$\mathbb{C}_n := \mathbb{C} \otimes \mathbb{R}_{p,q} = \{z = \sum_{A \subset N} z_A e_A : z_A \in \mathbb{C}\}.$$

The underlying (complex) vectorial space has obviously real dimension equal to $2n$. However, if a vector e_j in $\mathbb{C}_n$ satisfies $e_j^2 = +1$ then ie_j satisfies now $(ie_j)^2 = -1$. Therefore, the complex Clifford algebra $\mathbb{C}_n$ is no longer associated to an unique pair (p, q) but solely to the dimension $p + q = n$ of its associated (real-valued) vector space.

The (complex) conjugation of an arbitrary element $z = \sum_A z_A e_A \in \mathbb{C}_n$ is now defined as

$$\overline{z} = \sum_A \overline{z}_A \overline{e}_A,$$

where $\overline{z}_A$ corresponds to the usual complex conjugation and $\overline{e}_A$ is the conjugation in $\mathbb{R}_{p,q}$. For abuse of language we will make no distinction between both conjugations, the distinction being clear from the context.

Also, we have

$$z\overline{w} = \sum_{A,B\subset N} z_A \overline{w}_B e_A \overline{e}_B,$$

so we can define an inner product in $\mathbb{C}_n$ by

$$z|w := 2^n [z\overline{w}]_0, \tag{1.4}$$

and an associated norm in $\mathbb{C}_n$ as

$$|z|^2 := 2^n [z\overline{z}]_0 = 2^n \sum_A |z_A|^2 e_A \overline{e}_A = 2^n \sum_A |z_A|^2, \tag{1.5}$$

where $[\cdot]_0$ denotes the scalar part of the element.

1.1.3 Function spaces

In what follows, we consider $\Omega \subset \mathbb{R}^n$ a non-empty domain with piecewise smooth boundary $\Gamma = \partial\Omega$. A Clifford valued function $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}_{p,q}$ (resp., $\mathbb{C}_n$) can be written as $u(x) = \sum_A u_A(x) e_A$, where each u_A are real (resp. complex) valued functions in Ω.

A Clifford-valued function u is said to belong to a certain function space if and only if all its (real or complex valued) coordinate-functions u_A belong to the corresponding (real or complex) function space. For instance, $u = \sum_A u_A e_A$ belongs to $L_p(\Omega, \mathbb{C}_n)$ if and only if all its complex valued coordinate functions u_A are in $L_p(\Omega, \mathbb{C})$.

Whenever no confusion arises, the (Clifford valued) function spaces will be denoted by the same notation of its real counterparts, that is, $L_p(\Omega, \mathbb{C}_n)$ will be identified with $L_p(\Omega)$.

We now introduce the main functions spaces of Clifford valued functions, together with its norms and inner products (when existing).

For general (Clifford valued) L_p spaces, the usual norm is

$$||u||_{L_p} := \left(\int_\Omega |u(x)|^p \, dx \right)^{\frac{1}{p}} < \infty,$$

with $1 \leq p < \infty$. For $p \neq 2$ they are Banach spaces while $L_2(\Omega)$ is a Hilbert space, with inner product

$$< u, v >:= \int_\Omega u(x)|v(x) dx = 2^n \int_\Omega [u(x)\overline{v(x)}]_0 dx,$$

where $u, v \in L_2(\Omega)$.

We now define Sobolev spaces via Bessel potentials of the underlined functions. For $u = \sum_A u_A e_A$ we denote by $\hat{u} = \sum_A \hat{u}_A e_A$ its Fourier transform. We say that $u \in W_p^s(\Omega),\ s \in \mathbb{R},\ 1 \leq p < \infty$, if and only if

$$(1 + |\xi|^2)^{s/2} \hat{u}(\xi) \in L_p.$$

Remark: strictly speaking, the above spaces are in fact the spaces $H_p^s(\Omega)$, but for sufficiently smooth domains, i.e. Lipschitz domains, both spaces coincide (see [65]).

1.2 Clifford analysis

For a given boundary problem involving elliptic operators one can look for its solution in terms of single and double layer potentials. However, this method requires the explicit knowledge of a fundamental solution for the partial differential operator. In this section we will recall this type of approach, following closely the work of Gürlebeck and Sprößig in [39] for the analysis of the n-dimensional Laplace equation

$$\Delta u = \sum_{i=1}^{n} \partial_{x_i}^2 u.$$

In what follows, we will consider functions from (subsets of) $\mathbb{R}^n$ (conveniently identified with $\mathbb{R}^{0,n}$) into the real valued Clifford algebra $\mathbb{R}_{0,n}$.

1.2.1 Teodorescu operator

Let Ω be a domain in $\mathbb{R}^n$ with a piecewise smooth boundary $\Gamma = \partial\Omega$. We shall begin by introducing a first order operator which factorizes the n-dimensional Laplacian.

Definition 1.2.1 *Let $u \in C^1(\Omega)$. We define the Dirac operator as the first order operator*

$$Du(x) = (e_1 \partial_{x_1} + \cdots + e_n \partial_{x_n})\, u(x),$$

with $x \in \Omega$.

We have then that D factorizes the Laplacian, that is

$$\Delta v = -D^2 v,$$

for all $v \in C^2(\Omega)$.

We now present some results concerning a very special weakly singular integral operator, the Teodorescu operator, which plays a key role in the remaining of this thesis. For the proofs of the following results we refer to [39].

Definition 1.2.2 *Let $u \in C(\Omega)$. Then the linear integral operator*

$$Tu(x) = -\int_{\Omega} e(x-y)u(y)\ dy \tag{1.6}$$

is called the Teodorescu transform over Ω, where

$$e(x) = \frac{1}{\sigma_n}\frac{\overline{x}}{|x|^n}, \quad x = x_1e_1 + \cdots x_ne_n,$$

and σ_n denotes the surface area of a n-dimensional unit sphere.

The function e is such that $e(x) = DE(x)$, where $E(x) = \frac{1}{\sigma_n}\frac{1}{(2-n)}|x|^{-(n-2)}$ is the fundamental solution of the $n-$dimensional Laplace operator.

Next, we list some properties of this and related operators.

Lemma 1.2.3 *Let $u \in L_1(\Omega)$. Then the integral (1.6) exists for all $x \in \mathbb{R}^n$ and we have*

$$|Tu(x)| \leq \left(\frac{1}{\sigma_n}\max_{x\in\overline{\Omega}}\int_{\Omega}\frac{1}{|x-y|^{n-1}}\ dy\right)\ ||u||_{L_1(\Omega)}.$$

Now, we will present continuity results regarding to the operator T in the scale of Sobolev spaces.

Lemma 1.2.4 *The Teodorescu operator satisfies:*

(i) For $u \in C_0(\mathbb{R}^n)$, we have

$$\partial_{x_k}(Tu)(x) = -\frac{1}{\sigma}\int_{\Omega}\partial_{x_k}e(x-y)u(y)\ dy + \overline{e}_k\frac{u(x)}{n}.$$

(ii) The operator

$$\partial_{x_k}T : L_p(\mathbb{R}^n) \to L_p(\mathbb{R}^n)$$

is continuous and

$$||\partial_{x_k}T||_{L_p} \leq \left(C\sigma_n^{-\frac{1}{p}} + \frac{1}{n}\right), \quad 1 < p < +\infty.$$

(iii) If Ω is a bounded domain, then

$$T : L_p(\Omega) \to W_p^1(\Omega), \quad 1 < p < +\infty,$$

is continuous.

1.2.2 Clifford analysis using the Teodorescu operator

Based on the Teodorescu operator defined in the previous subsection and on some of its properties, we present the higher dimensional analogous of several classical theorems of complex analysis. Again, for the proofs we refer to [39].

Proposition 1.2.5 *Let $u \in C^2(\Omega) \cap C(\overline{\Omega})$. Then*

$$(DTu)(x) = \begin{cases} u(x) & \text{in } \Omega \\ 0 & \text{in } \mathbb{R}^n \setminus \overline{\Omega} \end{cases} .$$

Proposition 1.2.6 *Let $u, v \in C^1(\Omega) \cap C(\overline{\Omega})$, where Ω is a domain bounded by a Liapunov curve Γ. Then*

$$\int_\Omega [(uD)v + u(Dv)]\ dy = \int_\Gamma u(y)\alpha(y)v(y)\ d\Gamma_y,$$

where $(uD) = \sum_{i=1}^n (\partial_{x_i} u)e_i$, $Dv = \sum_{i=1}^n e_i(\partial_{x_i} v)$, and $\alpha(y)$ denotes the outward pointing normal vector at y.

Theorem 1.2.7 *Let $\Omega \subset \mathbb{R}^n$ be a domain which is bounded by a piecewise Liapunov surface Γ. Then, for $u \in C^1(\Omega) \cap C(\overline{\Omega})$ we have*

$$\int_\Gamma e(x-y)\alpha(y)u(y)d\Gamma_y - \int_\Omega e(x-y)(Du)(y)dy = \begin{cases} u(x) & , \ x \in \Omega \\ 0 & , \ x \notin \overline{\Omega} \end{cases} , \qquad (1.7)$$

where $\alpha(y)$ denotes again the outward pointing normal unit vector at y.

Definition 1.2.8 *Let $u \in C^1(\Omega) \cap C(\overline{\Omega})$. The operator F_Γ defined by*

$$(F_\Gamma u)(x) := \int_\Gamma e(x-y)\alpha(y)u(y)\ d\Gamma_y$$

is called Cauchy-Bitsadze operator.

Then formula (1.7) can be re-written as

$$(F_\Gamma u)(x) + (TDu)(x) = \begin{cases} u(x) & , \ x \in \Omega \\ 0 & , \ x \in \mathbb{R}^n \setminus \overline{\Omega} \end{cases} .$$

Theorem 1.2.9 ***(Cauchy's integral formula)*** *Let $\Omega \subset \mathbb{R}^n$ be a domain with a piecewise Liapunov boundary. Further, let $u \in \ker(D) \cap W_p^1(\Omega)$. Then*

$$(F_\Gamma u)(x) = \begin{cases} u(x) & in\ \Omega \\ 0 & in\ \mathbb{R}^n \setminus \overline{\Omega} \end{cases}$$

holds.

1.3 Laplace operators on manifolds

Until now we only have considered domains in $\mathbb{R}^n$ with the standard Euclidean Laplace operator $\Delta = \sum_{i=1}^{n} \partial_{x_i}^2$. We now look into more complex structures of manifolds endowed with an arbitrary metric. Hence, we introduce the Bochner-Laplacian and Günter-Laplacian, the operators which reflect the new metric structure.

1.3.1 The Minkowski metric

A pseudo-Riemannian metric on a smooth manifold M is a symmetric 2-tensor field g that is non-degenerate at each point $x \in M$. By far the most important pseudo-Riemannian metrics are the Lorentz metrics, which are pseudo-Riemannian metrics of index 1. The standard example of a Lorentz metric is the Minkowski metric, that is, a metric g on $\mathbb{R}^{n+1}$ that is written in terms of the local coordinates $(\xi_1, \ldots, \xi_n, \tau)$ as

$$g(d\overrightarrow{\xi}, d\overrightarrow{\xi}) = (d\xi_1)^2 + \ldots + (d\xi_n)^2 - (d\tau)^2. \tag{1.8}$$

In the special case of $\mathbb{R}^{3,1}$, the Minkowski metric is the fundamental invariant of Einstein's special theory of relativity, which can be expressed succinctly by saying that in the absence of gravity, the laws of physics have the same form in any coordinate system in which the Minkowski metric has the expression (1.8). The separation or difference of the physical characteristics of the space (the ξ directions) and time (the τ direction) arises from the fact that they are subspaces on which g is positive/negative definite, respectively.

1.3.2 Metric, tensors and vector bundles

Most of the technical machinery on Riemannian geometry is built up by means of tensors; indeed, a Riemannian metric itself is a tensor. Thus, we begin by reviewing the basic definitions and properties of tensors on a finite-dimensional vector space. When we put together spaces of tensors on a manifold, we obtain a particularly useful type of geometric structure called "vector bundle", which plays an important role in Section 2.2.

Let V be a finite-dimensional real vector space. As usual, V^* denotes the dual space of V - the space of covectors, or real-valued linear functionals, on V - and we denote the natural pairing $V^* \times V \to \mathbb{R}$ by either of the notations

$$(\omega, X) \mapsto < \omega, X > \qquad \text{or} \qquad (\omega, X) \mapsto \omega(X)$$

for $\omega \in V^*$, $X \in V$.

A covariant $k-$tensor on V is a multilinear map

$$F : \underbrace{V \times \ldots \times V}_{k\ copies} \to \mathbb{R}.$$

Similarly, a contravariant $l-$tensor is a multilinear map

$$F : \underbrace{V^* \times \ldots \times V^*}_{l\ copies} \to \mathbb{R}.$$

We often need to consider tensors of mixed types as well. A tensor of type (k, l), also called a $k-$covariant, $l-$contravariant tensor, is a multilinear map

$$F : \underbrace{V^* \times \ldots \times V^*}_{l\ copies} \times \underbrace{V \times \ldots \times V}_{k\ copies} \to \mathbb{R}.$$

The space of all covariant $k-$tensors on V is denoted by $T^k(V)$, the space of contravariant $l-$tensors by $T_l(V)$, and the space of mixed $(k, l)-$tensors is denoted by $T^k_l(V)$. The rank of a tensor is the number of arguments (vectors and/or covectors) it takes.

When we glue together the tangent spaces at all the points on a manifold M, we get a set that can be thought of both as a union of vector spaces and a manifold in its own right.

Definition 1.3.1 ***(see [48])*** *A smooth $k-$dimensional vector bundle is a pair of smooth manifolds E (the total space) and M (the base), together with the surjective map $\pi : E \to M$ (the projection), satisfying the following conditions:*

(a) *Each set $E_x := \pi^{-1}(x)$ (called the fiber of E over x) is endowed with the structure of vector space;*

(b) *For each $x \in M$, there is a neighborhood U of x and a diffeomorphism $\varphi : \pi^{-1}(U) \to U \times \mathbb{R}^k$, called local trivialization of E, such that the following diagram comutes:*

$$\begin{array}{ccc} \pi^{-1}(U) & \xrightarrow{\varphi} & U \times \mathbb{R}^k \\ \pi \downarrow & & \downarrow \pi_1 \\ U & = & U \end{array}$$

where π_1 is the projection onto the first factor.

(c) *The restriction of φ to each fiber, $\varphi : E_x \to \{x\} \times \mathbb{R}^k$, is a linear isomorphism.*

On a manifold M, we can perform the same linear-algebraic construction on each tangent space T_xM that we perform on any vector space, yielding tensors at x. For example, a $(k,l)-$tensor at $x \in M$ is just an element of $T^k_l(T_xM)$. We define the bundle of $(k,l)-$tensors on M as

$$T^k_l := \coprod_{x \in M} T^k_l(T_xM),$$

where $\coprod$ denotes the disjoint union. To see that this structure is a vector bundle, we define the projection $\pi : T^k_l M \to M$ to be the map that simply sends $F \in T^k_l(T_xM)$ to x.

We define a metric connection ∇ to be a connection in a Riemannian manifold equipped with a metric (M,g) for which the covariant derivatives of the metric on M vanish. Among other things, the metric property

$$Z\langle X, Y\rangle = \langle \nabla_Z X, Y\rangle + \langle X, \nabla_Z Y\rangle, \qquad X, Y, Z \in T_xM,$$

holds. This, in concert with

$$X^* = -X - \mathrm{div} X, \quad \forall X \in T_xM,$$

further entails that

$$(\nabla_X)^* = -\nabla_X - \mathrm{div} X, \quad \forall X \in T_xM.$$

For each $X \in T_xM$, ∇X is the tensor of type $(0,2)$ defined by

$$(\nabla X)(Y,Z) = \langle \nabla_Z X, Y\rangle, \qquad \forall Y, Z \in T_xM,$$

with trace

$$\mathrm{Tr}(\nabla X) = \sum_{j=1}^{n} \langle \nabla_{T_j} X, T_j\rangle = \mathrm{div} X,$$

for any orthonormal frame $\{T_j\}_j$ in T_xM.

As a special case, the Lévi-Civita connection is a metric connection which is torsion free. In this thesis we will endowed our Riemannian manifold with the Lévi-Civita connection ∇^g (also denoted, covariant derivative).

1.3.3 Bochner-Laplacian and Günter-Laplacian on manifolds

We give here the basic definitions from the theory of differential forms.

Definition 1.3.2 *Let M be a smooth manifold and T_xM its tangent space at the point x. The space $\bigwedge_k T_xM$ of differential $k-$ forms at x is the set of all $k-$linear alternating functions*

$$\omega : T_xM \times \cdots \times T_xM \to \mathbb{R}.$$

The space $\bigwedge_k T_xM$ is a vector space under the operations of addition and scalar multiplication. A $0-$form is a scalar, while the space $\bigwedge_1 T_xM$ of $1-$forms is the space of linear functions on T_xM, also denoted as cotangent space to M at x, that is, the dual vector space to the tangent space at x. If $\{x_1, \cdots, x_n\}$ are local coordinates, then T_xM has basis $\{\partial_{x_1}, \cdots, \partial_{x_n}\}$, while its dual cotangent space has (dual) basis $\{dx_1, \cdots, dx_n\}$.

A differential $1-$ form ω has the expression

$$\omega = f_1(x)dx_1 + \cdots + f_n(x)dx_n,$$

where each f_i is a smooth function. As operation rules we have $dx_i \wedge dx_j = -dx_j \wedge dx_i,\ i \neq j$, $dx_i \wedge dx_i = 0,\ i,j = 1, \ldots, n$. Moreover, the space $\bigwedge_k T_xM$ is spanned by the basic $k-$ forms

$$dx_A = dx_{i_1} \wedge \cdots dx_{i_k},$$

where $A = (i_1, \cdots, i_k),\ 1 \leq i_1 < \cdots < i_k \leq n$. Thus, $\bigwedge_k T_x M$ has dimension $\frac{n!}{(n-k)!k!}, k \leq n$, and any smooth differential $k-$form has local expression

$$\omega = \sum_A f_A(x) dx_A = \sum f_{i_1, \cdots, i_k}(x) dx_{i_1} \wedge \cdots dx_{i_k},$$

again f_A being smooth real valued functions. For more details, see [52].

Following [49], we now present the Laplace operator in the context of differential forms. The concept of harmonic function can be extended to differential forms as follows. Let $\star$ denotes the Hodge star operator, that is, a linear operator acting as

$$\star(1) = \pm dx_1 \wedge dx_2 \wedge \ldots \wedge dx_n,$$
$$\star(dx_1 \wedge dx_2 \wedge \ldots \wedge dx_n) = \pm 1,$$
$$\star(dx_1 \wedge dx_2 \wedge \ldots \wedge dx_p) = \pm dx_{p+1} \wedge \ldots \wedge dx_n,$$

where the $\pm$ sign corresponds to the positive/negative orientation of the form $dx_1 \wedge dx_2 \wedge \ldots \wedge dx_p$.

Using the exterior differentiation operator d, where

$$d(\sum_A f_A(x) dx_A) = \sum_A df_A(x) \wedge dx_A,$$

we introduce its adjoint d^* acting on $k-$forms by setting $d^* = (-1)^{n(p+1)+1} \star d \star$. Therefore, while the exterior differentiation operator maps $k-$forms into $(k+1)-$forms, its adjoint maps $k-$forms into $(k-1)-$forms. A $k-$form ω is said to be harmonic iff it is closed ($d\omega = 0$) and coclosed ($d^*\omega = 0$). We then introduce the Hodge Laplacian, also called Laplace-Beltrami operator, as $\Delta_H = d^*d + dd^*$.

There is another way to define a Laplacian, called Bochner-Laplacian, given by $\Delta_B = \nabla^*\nabla$, where ∇^* stands for the formal adjoint of the Lévi-Civita connection (for more details see [25]). This Laplacian and the Euclidean one introduced in Section 1.1 are related by the following special case of the Weitzenbock identity, proved in [34],

$$\nabla^*\nabla = -\Delta - \text{Ric}, \tag{1.9}$$

where Ric is the Ricci curvature on M. The Ricci curvature on M is a $(0,2)-$tensor defined as a contraction of $\mathcal{R}$

$$\mathrm{Ric}(X,Y)=\sum_{j=1}^{n}\langle\mathcal{R}(T_j,Y)X,T_j\rangle=\sum_{j=1}^{n}\langle\mathcal{R}(Y,T_j)T_j,X\rangle,\qquad \forall X,Y\in T_xM,$$

where $T_1,...,T_n$ is an orthonormal frame in T_xM, and $\mathcal{R}$ is the Riemann curvature tensor of M given by

$$\mathcal{R}(X,Y)Z=[\nabla_X,\nabla_Y]Z-\nabla_{[X,Y]}Z,\qquad X,Y,Z\in T_xM,$$

with $[X,Y]=XY-YX$ is the usual commutator bracket. Thus, Ric is a symmetric bilinear form.

It is know that one possible extension of the most basic partial differential operators on an domain $M\subset\mathbb{R}^n$, can be expressed globally, in terms of the standard spatial coordinates in $\mathbb{R}^n$. It turns out that a convenient way to carry out this program is by employing the so-called Günter derivatives (for more details see [25] and [36])

$$\mathcal{D}:=(\mathcal{D}_1,\mathcal{D}_2,...,\mathcal{D}_n),\tag{1.10}$$

where for each $1\leq j\leq n$, the first-order differential operator $\mathcal{D}_j$ is the directional derivative along ψe_j, where $\psi:\mathbb{R}^n\to T_xM$ is the orthogonal projection onto the tangent plane to M and, as usual, $e_j=(\delta_{j,k})_{1\leq k\leq n}\in\mathbb{R}^n$, with δ_{jk} denoting the Kronecker symbol. The operator $\mathcal{D}$ is globally defined on M by means of the unit normal vector field, and has a relatively simple structure. In terms of (1.10), the Laplace operator defined via Günter derivatives, namely Günter-Laplacian, becomes

$$\Delta_G=\mathcal{D}^2=\sum_{j=1}^{n}\mathcal{D}_j^2=\sum_{j=1}^{n}(\partial_{x_j}-\nu\partial_\nu)(\partial_{x_j}-\nu\partial_\nu),$$

with $\nu(x):=\frac{x}{||x||}$, $x\in\mathbb{R}^n\setminus\{0\}$, and $\partial_\nu=\sum_{j=1}^{n}\left(\frac{x_j}{||x||}\right)\partial_{x_j}$ be the radial derivative in $\mathbb{R}^n$. For the Laplace operator introduced in Section 1.1 and Δ_G is valid the following identity

$$\Delta=\psi\mathcal{D}^2+2R^2-\mathcal{G}R,\tag{1.11}$$

where $R(x)=\nabla\nu(x)$ and $\mathcal{G}=\mathrm{div}\nu$. Relations (1.10) and (1.11) are proved in [25].

Chapter 2

The Schrödinger problem

"In my paper the fact that XY was not equal to YX was very disagreeable to me.
I felt that this was the only point of difficulty with the whole scheme."
Werner Heisenberg

The theory of partial differential equations on surfaces stems from the intensive study of a few special equations, whose importance was recognized in the eighteenth and nineteenth centuries, known as basic equations in mathematical physics (gravitational, electromagnetism, sound propagation, heat transfer and quantum mechanics). It was shown that these equations play important roles in almost all fields of science, for instance, the Laplace equation was initially studied as the basic equation in the theory of Newton's potential and in electrostatic, and later it was used to study geometry and topology of Riemannian manifolds. The heat equation was initially studied in the context of heat transfer, and later it was shown to be related to the probability theory, heat conduction on surfaces, shell problems in elasticity, or Navier-Stokes equations.

One of the most important PDE's is the Schrödinger equation. Physically, this equation describes the space and time dependence of quantum mechanical systems. It is of extreme importance to the theory of quantum mechanics, playing a role analogous to Newton's second law in classical mechanics. In mathematical formulation of quantum mechanics, each system is associated with a complex Hilbert space such that each instantaneous state of the system is described by a unit vector in that space. This state vector encodes the probabilities for the outcomes of all possible measurements applied to the system. As the state of a system generally changes over time, the state vector is a function of time. The Schrödinger equation provides a quantitative description of the rate of change of the state vector.

Formally, the Schrödinger equation is

$$H(x)\psi(x,t) = \pm i\hbar\partial_t\psi(x,t),$$

where i is the imaginary unit, x the space-variable, t the time-variable, ∂_t is the partial derivative with respect to t, $\hbar$ is the reduced Planck's constant (Planck's constant divided by 2π), $\psi(x,t)$ is the wave function, $H(x)$ is the Hamiltonian (self-adjoint operator acting on the space variable), and $\pm$ represents the forward/backward case, respectively.

The Hamiltonian describes the total energy of the system. As with the force occurring in the Newton's second law, its exact form is not provided by the Schrödinger equation, and must be independently determined based on the physical properties of the system.

In order to simplify the calculations over the thesis we will omit the reduced Planck's constant, and in order to avoid blow-up problems in future numerical implementations we will concentrate in the backward case.

There are several areas of Mathematics that can be applied in the study of PDE's. However, most of them are only efficient when we are dealing with elliptic operators, failing for the case of parabolic and hyperbolic operators, as for example, in the case of the Schrödinger operator or the heat operator. In this chapter, we will try to apply some of the elliptic techniques used to study the heat problem in the analysis of the Schrödinger problem. However, we need to take into account that in many aspects the Schrödinger operator is substantially different from the heat one: the Galilean group is the invariance group associated to the first equation, while the parabolic group is the invariance group associated to the heat equation (for more details see [64]). Also, the Schrödinger equation is related to the Minkowski space-time metric, while the heat equation is linked to the parabolic space-time metric. More important for us, in an analytical point of view, the singularity $t = 0$ of the correspondent fundamental solutions is removable outside the origin in the second case but not in the Schrödinger case. This force us to introduce a regularization procedure prior to the treatment by semigroup theory or hypoelliptic theory.

Here, we consider two approaches ($K-$theory combined with semigroup theory and hypoelliptic theory) that allows a successful resolution of the linear regularized Schrödinger problem. Since we want to do a numerical implementation of the theoretical results, we will verify that these two traditional approaches are not the most suitable for our purposes.

In more detail, the implementation of $K-$theory is connected with the concepts of vector bundle, differential forms and the construction of the regularized Schrödinger semigroup (Section 2.2). As to the hypoelliptic theory, we will construct the parametrix associated to the regularized Schrödinger operator (Section 2.3). We remark that in the first approach we will extend our results to other "Schrödinger type" operators where, in order to study non-flat manifolds, the Euclidean-Laplacian is replaced by the Bochner-Laplacian and the Günter-Laplacian.

In both approaches we will make some observations about the behavior of our results in the limit case

2.1 Regularization of the non-stationary Schrödinger operator

It is well-known that fundamental solutions of the time dependent Schrödinger operator have non-removable singularities in whole of the hyperplane $t = 0$ and, therefore, one cannot use directly methods of hypoelliptic operators. This carries additional problems for the study of the arising integral operators, where we cannot guarantee the convergence, in the classical sense, of the integrals that define those operators.

In order to solve this problem we need to regularize the fundamental solution and the arising operators (see [64]). This process of regularization creates a family of operators and correspondent fundamental solutions, which are locally integrable in $\mathbb{R}^n \times \mathbb{R}_0^+ \setminus \{(\underline{0}, 0)\}$. Moreover, this family will converge to the original operators and fundamental solution when $\epsilon \to 0^+$.

To this end, we will replace the imaginary unit in the Schrödinger operator by $\mathbf{k} = \dfrac{\epsilon + i}{\epsilon^2 + 1}$ and we obtain the operator $-\Delta \pm \mathbf{k}\partial_t$. For each $\epsilon > 0$, $-\Delta \pm \mathbf{k}\partial_t$ is a hypoelliptic operator, in the sense of Theorem A.2.3 and, therefore, we have ensured the good behavior of the associated integral operators. More details about the regularization of the Schrödinger operator will be presented in Subsection 3.2.1.

2.2 Approach via semigroup theory

The use of semigroup theory to study partial differential equations is not new. In the case of time dependent operators, like the heat or the Schrödinger, one usually use the Laplace operator as a formal generator for the stationary part and use the form perturbation theory presented by Voigt [68] in order to construct the semigroup associated to the desired second order operator.

The main results presented in this section are based in Eichhorn's ideas (see [28]). In his paper the author presents the heat semigroup acting either on tensors or differential forms, with values in a vector bundle and applies it to solve the heat problem with initial data. Taking into account the regularization process described in the previous section, we will extend the existing results for the heat semigroup to the regularized Schrödinger operator.

As we will see, the application of the $K-$theory combined with the semigroup theory allows the deduction, in a simple and practical way, of existence and uniqueness results for the linear regularized Schrödinger problem with initial condition. However, we cannot present explicit expressions for this solution, which creates problems for future numerical implementation.

2.2.1 Basic notions in semigroup theory

Consider an operator $F : D_F \subset X \to X$ with D_F dense in X an F a closed operator. First we introduce the following characterization of a normalized tangent functional via the complex version of the Hahn-Banach theorem (for more details see [33]).

Theorem 2.2.1 *Let X be a complex Banach space and Y be a linear subspace of X. If $u \in Y^*$, then there exist a normalized tangent functional $u^* \in X^*$ such that $u^*|_Y = u$ and $||u^*||_{X^*} = ||u||_{Y^*}$.*

The previous characterization is equivalent to the characterization present by Yosida (see [69], page 106).

Taking into account the previous result, F is said to be dissipative if for every $u \in D_F$ there exists a normalized tangent functional such that $\langle u^*, Fu\rangle \leq 0$. The closure of a dissipative operator is dissipative. For the particular case of X being a Hilbert space and F a symmetric operator, if $\langle Fu, u\rangle \leq 0$ for all $u \in D_F$ then F is dissipative. We say that C^0-semigroup

$\{T_t\}_{t\in\mathbb{R}_0^+}$ of bounded linear operators $T_t \in L(X,X)$, where X is a Banach space, is called a contraction semigroup if $||T_t|| \leq 1$, for $0 \leq t < +\infty$. The infinitesimal generator F of a semigroup $\{T_t = e^{Ft}\}_{t\in\mathbb{R}_0^+}$ is defined by

$$F := \lim_{t\to 0^+} \frac{T_t - I}{t}.$$

For more details see [69]. During this section, we will consider the following alternative characterization of the infinitesimal generator of a semigroup.

Lemma 2.2.2 ***(c.f. [55])*** *The operator $A : D_A \to X$, with D_A dense and close, is the infinitesimal generator of a contraction semigroup if and only if A is dissipative and* $\mathrm{Range}(\mu - A) = X$*, for some $\mu > 0$.*

2.2.2 The regularized Schrödinger operator acting on vector bundles

In this subsection we study the action of the regularized Schrödinger semigroup over vector bundles. The main objective is to construct the regularized semigroup associated to our operator, namely $\{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$, and to show that, under specific values of p, we can use it to obtain a unique solution of the regularized Schrödinger equation in L_p. The application to the resolution of the equation will only possible after we study the dissipativity of the elements of the semigroup.

Across the rest of this section, we will consider (M, g) a (complete) Minkowski manifold and $(\mathbb{C}, M, \pi)$ a vector bundle with an associated metric connection ∇^π. The Lévi-Civita connection ∇^g and the metric connection ∇^π induces a metric connection ∇ in all tensor bundles $\mathcal{T}_q^r \otimes \mathbb{C}$ over M. For $1 \leq p < +\infty$, let $L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ be the Banach space of all measurable $(r,q)-$tensors u with values in $\mathbb{C}$ such that

$$||u||_p = \left(\int_M |u|^p \ d\mu_g \right)^{\frac{1}{p}} < \infty,$$

where $d\mu_g$ is the measure induced by the metric g. Here $L_p^0(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ will denote the elements of $L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ with compact support. For $p = 2$, $L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ corresponds to the usual Hilbert space.

Let $L_p(\bigwedge_k T_x M \otimes \mathbb{C})$ be the corresponding space of $k-$forms with values in $\mathbb{C}$ and $L_p^0(\bigwedge_k T_x M \otimes \mathbb{C})$ of those with compact support.

Semigroup associated to regularized Schrödinger operators

The use of the semigroups techniques in the study of time-evolution equations has several advantages. For example, they provide an elegant alternative to some of the existence theory of evolution equations. The connections between semigroup theory and the Schrödinger equation were developed by many authors, e.g. in [70] where the author constructed the associated semigroup via the infinitesimal generator. This approach do not requires any type of regularization procedure and do not use the spectral theorem. However, in our case this construction will not be so direct and immediate.

Here, as we refer previously, we want to construct, in a simplest possible way, the semigroup associated to our evolution operator. This construction is based in the ideas presented in [28] by Eichhorn. The main difference between his and our approach is that we cannot use the Schrödinger operator itself. This impossibility is due to the fact that our time-dependent operator is not hypoelliptic. Hence we will only be able to construct one semigroup for each element of the family of hypoelliptic operators $-\Delta - \mathbf{k}\partial_t$, where we recall $\mathbf{k} = \frac{\epsilon+i}{\epsilon^2+1}, \epsilon > 0$.

On open and complete manifolds the Laplace operator, with respect to the L_2-norm, is essentially self-adjoint on tensors fields with compact support. Taking into account the regularization procedure described in Subsection 2.1, we obtain, applying the spectral theorem (for more details about its application to the Dirac operator in the context of Clifford analysis see [22]), we obtain the following integral operator

$$\Gamma_t^{\mathbf{k}} = \int_0^{+\infty} e^{-\mathbf{k}t\lambda}\, dE_\lambda,$$

which, for each $\mathbf{k}$ and t fixed, verifies the following properties:

(i) it is well defined in $L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$;

(ii) for $u \in L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$, we have $(-\Delta - \mathbf{k}\partial_t)\Gamma_t^{\mathbf{k}} u = \Gamma_t^{\mathbf{k}}(-\Delta - \mathbf{k}\partial_t)u$;

(iii) for $u \in L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$, the mapping $t \mapsto \Gamma_t^{\mathbf{k}} u$ is differentiable;

(iv) for $u \in L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$, we have $\partial_t \Gamma_t^{\mathbf{k}} u = (-\Delta - \mathbf{k}\partial_t)\Gamma_t^{\mathbf{k}} u$.

These properties follow immediately from differential properties of semigroups and can be found in [29], page 414.

Dissipative property of the regularized operators

Now we want to verify if the elements of the regularized semigroup $\{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$ are dissipative. This property of the elements of the regularized semigroup is very important because it will give us the possibility of obtain better results of solutions to initial-value problems.

To do that we first prove that, for each fixed $\mathbf{k}$, the elements of the semigroup satisfy the conditions of Lemma 2.2.2, i.e, $\text{Range}(\mu - (-\Delta)) = X$, for some $\mu > 0$, or equivalent $\text{Range}(\mu - \Delta) = X$, for some $\mu < 0$.

Lemma 2.2.3 *Let M be a Minkowski manifold. Suppose that $u \in L_p(\mathcal{T}_q^r(M)\otimes\mathbb{C})+L_q(\mathcal{T}_q^r(M)\otimes\mathbb{C})$, with $1 < p \leq q < 3$ and*

$$-\Delta u = \mu u,$$

for some $\mu > 0$. Then u is identically zero.

For the proof we remark that this Lemma corresponds to Lemma 3.2 in [28] where also the proof is given.

In these conditions, we immediately obtain the main result of this subsubsection.

Lemma 2.2.4 *$-\Delta$ is dissipative on $L_p^0(\mathcal{T}_q^r(M)\otimes\mathbb{C})$, for $1 < p < 3$.*

Proof: If $u \in L_p^0(\mathcal{T}_q^r(M)\otimes\mathbb{C})$ then

$$\begin{aligned}\langle |u|^{p-2}u, -\Delta u\rangle &= \langle D(|u|^{p-2}u), Du\rangle \\ &= \langle |u|^{p-2}\, Du, Du\rangle + (p-2)\langle |u|^{p-3}(uDu), Du\rangle.\end{aligned}$$

Then

$$\begin{aligned}0 \leq \left|\langle |u|^{p-3}(uDu), Du\rangle\right| &\leq \int_M |u|^{p-3}\,|u|\,|Du|\,|Du|\,d\mu_g \\ &= \langle |u|^{p-2}\, Du, Du\rangle,\end{aligned}$$

i.e., with $|p-2| < 1$

$$\langle |u|^{p-2}u, -\Delta u\rangle \leq 0.$$

■

Main result

The aim of this subsubsection is to determinate for which values of p the property $u \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ implies the unicity of the associated semigroup $\{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$ and that $\Gamma_t^{\mathbf{k}} u$ is a solution of the regularized Schrödinger equation.

Theorem 2.2.5 *Consider M a Minkowski manifold. Consider also $(\mathbb{C}, \pi, M)$ a vector bundle. Denote by $\{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$ the regularized Schrödinger semigroup acting on $L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$. Then $||\Gamma_t^{\mathbf{k}} u||_p \leq ||u||_p$, for all $u \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C}) \cap L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ and $\frac{3}{2} < p < 3$.*

Therefore, $\{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$ extends to a contraction semigroup on $L_p^0(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ for $\frac{3}{2} < p < 3$. Moreover, $\Gamma_t^{\mathbf{k}} u$ satisfies the regularized Schrödinger equation

$$\mathbf{k}\partial_t(\Gamma_t^{\mathbf{k}} u) = -\Delta(\Gamma_t^{\mathbf{k}} u),$$

for $u \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ and $\{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$ is unique.

Proof: The closure A of $-\Delta|_{L_p^0(\mathcal{T}_q^r(M)\otimes\mathbb{C})}$ in $L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ is dissipative for $1 < p < 3$.

Furthermore, $\mu - A$ is surjective for $\mu > 0$ and the above p. In fact, if this would not be the case there would exist an $u \in L_{p'}(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ such that $\langle u, (\mu - A)v \rangle = 0$, for all $v \in L_p^0(\mathcal{T}_q^r(M) \otimes \mathbb{C})$. This would imply $\Delta u = -\mu u$, for $\mu > 0$, and contradicting Lemma 2.2.2.

From $p' < 3$ we get the restriction $p > \frac{3}{2}$. Hence, A generates a contraction semigroup $\{Q_t\}_{t\in\mathbb{R}_0^+}$ for $\frac{3}{2} < p < 3$.

Next, we show that the semigroups Q_t and $\Gamma_t^{\mathbf{k}}$ agree on

$$L_2 \cap L_p = L_2(\mathcal{T}_q^r(M) \otimes \mathbb{C}) \cap L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C}).$$

For this it is sufficient to show that $(\mu - (-\Delta))^{-1}$ and $(\mu - A)^{-1}$ coincide on $L_2 \cap L_p$. Suppose that $u \in L_2 \cap L_p$, $(\mu - (-\Delta))^{-1} u = v$, $(\mu - A)^{-1} u = w$. Then $v \in L_2$, $w \in L_p$, $v - w \in L_2 + L_p$ and $\Delta(v - w) = -\mu(v - w)$, $\mu > 0$. According to Lemma 2.2.3, we have $v = w$, $\{Q_t\}_{t\in\mathbb{R}_0^+} = \{\Gamma_t^{\mathbf{k}}\}_{t\in\mathbb{R}_0^+}$ on $L_2 \cap L_p$.

This proves the estimate $||\Gamma_t^{\mathbf{k}} u||_p \leq ||u||_p$, for $\frac{3}{2} < p < 3$.

Since $\Gamma_t^{\mathbf{k}} u$ satisfies the regularized Schrödinger equation for $u \in D_\Delta$ (c.f. Lemma 2.2.2) and since this domain is dense in $L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$, $\Gamma_t^{\mathbf{k}} u$ also satisfies the regularized Schrödinger equation, but at the first instance only in distributional sense. The hypoellipticity of the regularized Schrödinger operator implies this in the pointwise sense.

Now, we prove the uniqueness. If A' is the infinitesimal generator of another contraction semigroup $\{P_t\}_{t\in\mathbb{R}_0^+}$, such that P_tu satisfies the regularized Schrödinger equation, then we have to show $(\mu - A')^{-1} = (\mu - (-\Delta))^{-1}$.

We have $(\mu - A')^{-1}u = v$ which means $v \in D_A$, and $(\mu - A')v = u$. If $v \in D_A$, then

$$t^{-1}(P_tv - v) \quad \to \quad L'v \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C}),$$

$$t^{-1}(P_{s+t}v - P_sv) \quad \to \quad P_sA'v \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C}),$$

for any fixed $s > 0$. P_tu satisfies the regularized Schrödinger equation. Therefore

$$t^{-1}(P_{s+t}v - P_sv) \to \partial_sP_sv = -\Delta P_sv,$$

i.e., $P_sA'v = -\Delta P_sv$. Then

$$A'v = \lim_{s\to 0}(-\Delta P_sv) = -\Delta v$$

in the distributional sense. It follows $v \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ satisfies $(\mu - (-\Delta))v = u$. On the other hand, if $(\mu - (-\Delta))^{-1}u = w$, then $w \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$ and

$$(\mu - (-\Delta))w \quad = \quad u,$$

$$\Delta(v - w) \quad = \quad -\mu(v - w), \quad \mu > 0.$$

According to Lemma 2.2.3, $v = w$, and consequently we obtain our result.

■

Laplacian for manifolds

The classical Laplace operator is not suited for arbitrary manifolds, since it fails to take into consideration its underlined geometric structure, e.g. its curvature or its non-Riemmanian metric. Hence, we aim now to extend some of the previous results to a Schrödinger-type operator where the Laplace operator is replaced by the Bochner-Laplacian or by the Günter-Laplacian. For that, we shall write these equations in local cartesian coordinates and associated differential forms rather than using intrinsic metric tensor coordinates.

The representation via differential forms is simpler than the representation based on the classical covariant $g = [g_{jk}]_{(n-1)\times(n-1)}$ and contravariant $g^{-1} = [g^{jk}]_{(n-1)\times(n-1)}$ Riemannian metric tensors on a manifold M. Moreover, they have the advantage of fit naturally into integral formulation, since they provide immediate linkage between local and global geometry (topology) and unlike tensors differential forms do not need indices, i.e., they do not have to be written in terms of components, thus simplifying the arising expressions.

In the case of the Bochner-Laplacian we need to impose $\mathrm{Ric} > 0$ while for the Günter-Laplacian we require $2R^2 - \mathcal{G}R > 0$. With these additional conditions and taking into account (1.9) and (1.11), we can establish analogous proofs to the previous results and we have that:

- The operators $-\Delta_B$ and $-\Delta_G$ with domain $L^0_p(\bigwedge_k T_xM \otimes \mathbb{C})$ are dissipative for $1 < p < 3$.
- $||\Gamma^{\mathbf{k}}_t u||_p \leq ||u||_p$, for all $u \in L_p(\bigwedge_k T_xM \otimes \mathbb{C}) \cap L_2(\bigwedge_k T_xM \otimes \mathbb{C})$ and $\frac{3}{2} < p < 3$ and, therefore, $\{\hat{\Gamma}^{\mathbf{k}}_t\}_{t\in\mathbb{R}^+_0}$ extends to a contraction semigroup on $L^0_p(\bigwedge_k T_xM \otimes \mathbb{C})$ for $\frac{3}{2} < p < 3$.

2.2.3 The regularized Schrödinger problem

In this subsection, we show how the Schrödinger semigroup $\{\Gamma^{\mathbf{k}}_t\}_{t\in\mathbb{R}^+_0}$ relates to the initial boundary problem for the regularized Schrödinger equation $(-\Delta - \mathbf{k}\partial_t)u = 0$. Initially, we consider the case of the regularized operator acting on vector bundles after which we generalize our conclusions to the cases of the Bochner-Laplacian and the Günter-Laplacian. Taking into account Theorem 2.2.5, we immediately obtain

Theorem 2.2.6 *Let M be a Minkowski manifold and $\frac{3}{2} < p < 3$. Then the initial value problem*

$$\begin{cases} (-\Delta - \mathbf{k}\partial_t)v = 0, & \text{on } M \times \mathbb{R}^+ \\ v(x,0) = u_0(x), & \text{on } M \end{cases} \tag{2.1}$$

is solvable, with $v(\cdot, t) \in L_p(\mathcal{T}^r_q(M) \otimes \mathbb{C})$, whenever $u_0 \in L_p(\mathcal{T}^r_q(M) \otimes \mathbb{C})$.

The remaining open question of uniqueness is answered in the following result

Theorem 2.2.7 *Let M be a Minkowski manifold and $\frac{3}{2} < p < 3$, $v = v(x,t)$ a solution of the regularized Schrödinger equation with $v(\cdot,t) \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$. Assume further $||v(\cdot,t)||_p \leq ae^{-|\mathbf{k}|bt}$. Then there exists a uniquely determined $u_0 \in L_p(\mathcal{T}_q^r(M) \otimes \mathbb{C})$, such that $v = \Gamma_t^{\mathbf{k}} u_0$.*

Proof: In the following proof we denote the corresponding space solution by L_p.

If $u_0 = \lim_{t_j \to 0} v(\cdot, t_j)$ in the weak star topology, $u = v - \Gamma_t^{\mathbf{k}} u_0$, then

$$||u(\cdot,t)||_p \leq ae^{-|\mathbf{k}|bt} \tag{2.2}$$

and

$$u(\cdot, t_j) \to 0, \quad \text{when } t_j \to 0 \tag{2.3}$$

in the distributional sense.

Furthermore, u satisfies the regularized Schrödinger equation since each term does. We have to show that $u = 0$. To do this we consider the Laplace transform of u

$$w_\lambda^{\mathbf{k}}(x) = \int_0^{+\infty} e^{-|\mathbf{k}|t\lambda} u(x,t)\, dt.$$

According (2.2) the integral converges absolutely for sufficiently large $|\mathbf{k}|\lambda$ and almost all x. Moreover, $w_\lambda^{\mathbf{k}} \in L_p$. Next we show $\Delta w_\lambda^{\mathbf{k}} = -\mathbf{k}\lambda w_\lambda^{\mathbf{k}}$ in the distributional sense. For any $\psi \in L_p^0(\mathcal{T}_q^r(M) \otimes \mathbb{C})$

$$\begin{aligned} \langle \psi, \Delta w_\lambda^{\mathbf{k}} \rangle &= \langle \Delta\psi, w_\lambda^{\mathbf{k}} \rangle \\ &= \int_0^{+\infty} e^{-|\mathbf{k}|t\lambda} \langle \Delta\psi, u(\cdot,t) \rangle\, dt. \end{aligned} \tag{2.4}$$

According to (2.2) the previous double integral converges absolutely for large $|\mathbf{k}|\lambda$. Using the regularized Schrödinger equation

$$\langle \Delta\psi, u(\cdot,t) \rangle = -\mathbf{k}\partial_t \langle \psi, u(\cdot,t) \rangle,$$

we obtain via integration by parts

$$
\begin{aligned}
\langle \psi, \Delta w_\lambda^{\mathbf{k}} \rangle &= -\int_0^{+\infty} e^{-|\mathbf{k}|t\lambda} \partial_t \langle \psi, u(\cdot,t)\rangle \; dt \\
&= - \lim_{\substack{t_j \to 0 \\ N \to +\infty}} \int_{t_j}^{N} e^{-|\mathbf{k}|t\lambda} \partial_t \langle \psi, u(\cdot,t)\rangle \; dt \\
&= - \lim_{\substack{t_j \to 0 \\ N \to +\infty}} \Big[\lambda \int_{t_j}^{N} e^{-|\mathbf{k}|t\lambda} \langle \psi, u(\cdot,t)\rangle \; dt + e^{-|\mathbf{k}|N\lambda} \langle \psi, u(\cdot,N)\rangle \\
&\qquad\qquad - e^{-|\mathbf{k}|t_j\lambda} \langle \psi, u(\cdot,t_j)\rangle \Big] \\
&= -\lambda \int_0^{+\infty} e^{-|\mathbf{k}|t\lambda} \langle \psi, u(\cdot,t)\rangle \; dt
\end{aligned}
$$

since $e^{-|\mathbf{k}|N\lambda}\langle \psi, u(\cdot,N)\rangle$ by (2.2) and $e^{-|\mathbf{k}|t_j\lambda}\langle \psi, u(\cdot,t_j)\rangle$ by (2.3).

Altogether $\Delta w_\lambda^{\mathbf{k}} = -\mathbf{k}\lambda w_\lambda^{\mathbf{k}}$ in the distributional sense. Now $w_\lambda^{\mathbf{k}} = 0$ by Lemma 2.2.3. From the uniqueness of the complex Laplace transform we conclude that $u = 0$ a.e.

If $v = e_-^{\epsilon} u_0'$, then

$$||u_0 - u_0'|| \le ||e_-^{\epsilon} u_0' - u_0'|| + ||u_0 - e_-^{\epsilon} u_0|| + ||e_-^{\epsilon} u_0 - e_-^{\epsilon} u_0'||. \tag{2.5}$$

The first two terms tend to zero if $t \to 0$, the third term equals to zero by hypothesis. Hence $u_0' = u_0$.

■

Remark 2.2.8 *As we saw, the semigroup theory provides an elegant method for establishing existence and uniqueness results for the regularized Schrödinger problem. However, it is important to remark that the application of this theory was only possible since the coefficients are time-independent. In the case where the coefficients of the operator are time-dependent we would need to implement a Galerkin method (for more details see Section 7.1, [29]).*

As in Subsection 2.2.2, we can extend the previous results to the case a setting of differential forms. Also here, we will need to impose additional technical conditions concerning the positiveness of the curvatures of the manifold M.

In the case of differential forms we need to impose that $\mathrm{Ric} > 0$ and in the case of the Günter derivatives $2R^2 - \mathcal{G}R > 0$. With this two additional conditions and taking into account the relations (1.9) and (1.11), we can establish analogous proof and conclude that in the case of differential forms the regularized Schrödinger problem is solvable when $v(\cdot, t) \in L_p(\bigwedge_k T_xM \otimes \mathbb{C})$ and $u_0 \in L_p(\bigwedge_k T_xM \otimes \mathbb{C})$, with $\dfrac{3}{2} < p < 3$. Let us observe that the restrictions imposed to the function v are consequence of the conclusions obtained in Subsection 2.2.2.

It remains to study the behavior of the conclusions obtained in this section when $\epsilon \to 0$. Taking into account the ideas presented in [17] regarding the convergence of the solutions of the regularized Schrödinger problem when $\epsilon \to 0$ and the fact that $(-\Delta - i\partial_t)^{-1}$ exists and it is unique (see [66]), we can extend our existence results to the discussed settings. Uniqueness is ensured in these settings by absolutely convergence when $\epsilon \to 0$.

2.3 Parametrix and hypoelliptic theory

The aim of this section is to implement hypoelliptic theory in the construction of the parametrix associated to the regularized Schrödinger operator. At the end of the section we show that this approach allows not only to obtain existence and uniqueness results, but also presents an explicit expression for the solution of the Schrödinger problem. However, this representation is too dependent on the choice of the parameter ϵ used in the regularization procedure. This problem being ill-posed, it increases the difficulties of the numerical implementation. In fact, the dependence on ϵ makes the algorithm very unstable for small values of the parameter ϵ .

Decomposition of Pseudodifferential Operators of order 2

From now on, we consider $\Omega = \underline{\Omega} \times [0, T) \subset \mathbb{R}^n \times \mathbb{R}_0^+$, a open (non-empty) domain with a piecewise smooth boundary and $\Gamma = \partial\Omega$. We can assume that $-\Delta \pm \mathbf{k}\partial_t$ is also a pseudodifferential operator with principal symbol in the Hörmander class $S^0_{1,0}$. (for more details see [42]).

The total symbol of $-\Delta \pm \mathbf{k}\partial_t$ is

$$P_{\mathbf{k}}(x,t,\xi,\tau) := P_{\mathbf{k}}(\xi,\tau) = -|\xi|^2 \pm i\mathbf{k}\tau,$$

where $x = (x_1, \dots, x_n)$, $\xi = (\xi_1, \dots, \xi_n)$ and $|\xi|^2 = \xi_1^2 + \dots + \xi_n^2$.

In our particular case, condition (H2) (see Theorem A.1.2) guarantees that the symbol $P_{\mathbf{k}}(x,t,\xi,\tau)$ is not singular. This allows us to conclude that all the elements of the family $-\Delta \pm \mathbf{k}\partial_t$, with symbol $P_{\mathbf{k}}(\xi,\tau)$, are invertible modulo regularizing operators. Moreover, condition (H2) implies that for each compact $K \subset \Omega$ the total symbol $P_{\mathbf{k}}(\xi,\tau)$, as a polynomial of degree 2 in $|\xi|$, has no real zeros for $|\tau|$ large. Therefore, when $|\tau| > M$, $P_{\mathbf{k}}(\xi,\tau)$ will have the following complex roots

$$z_1 = z_1(\tau) = \sqrt{\pm i\mathbf{k}\tau} \qquad\qquad z_2 = z_2(\tau) = -\sqrt{\pm i\mathbf{k}\tau}.$$

Consequently,

$$P_{\mathbf{k}}(\xi,\tau) = P_{\mathbf{k}}^{-}(\xi,\tau)\ P_{\mathbf{k}}^{+}(\xi,\tau),$$

where

$$\begin{aligned} P_{\mathbf{k}}^{-}(\xi,\tau) &= (|\xi| - z_2(\tau)) = (|\xi| + \sqrt{\pm i\mathbf{k}\tau}), \\ P_{\mathbf{k}}^{+}(\xi,\tau) &= (|\xi| - z_1(\tau)) = (|\xi| - \sqrt{\pm i\mathbf{k}\tau}), \end{aligned} \tag{2.6}$$

for $(x,t) \in K$, $|\tau| > M$.

In the rest of this subsection, we will consider only the backward case.

Theorem 2.3.1 *Consider the operator $-\Delta - \mathbf{k}\partial_t$ and its total symbol $P_{\mathbf{k}}(\xi,\tau)$. There exists a pseudodifferential operator $L_{\mathbf{k}}$ invertible modulo regularizing operators, such that*

$$-\Delta - \mathbf{k}\partial_t = L_{\mathbf{k}}(\partial_x,\partial_t) P_{\mathbf{k}}^{-}(\partial_x,\partial_t) P_{\mathbf{k}}^{+}(\partial_x,\partial_t) + R_{\mathbf{k}}(\partial_x,\partial_t), \tag{2.7}$$

where $R_{\mathbf{k}}$ is a regularizing term, where $\partial_x = (\partial_{x_1}, \dots, \partial_{x_n})$.

Proof: Assume that $P_{\mathbf{k}}(\xi,\tau)$, as well as $P_{\mathbf{k}}^{\pm}(\xi,\tau)$, satisfy conditions (H1) and (H2). According to [7], we can construct the following first order operators $K_{\mathbf{k}}^{\pm}(\partial_x,\partial_t)$

$$K_{\mathbf{k}}^{\pm}(\partial_x,\partial_t) = \partial_t + P_{\mathbf{k}}^{\pm}(\partial_x,\partial_t),$$

where $P_{\mathbf{k}}^{\pm}(\partial_x, \partial_t)$ are pseudodifferential operators with symbol $P_{\mathbf{k}}^{\pm}(\xi, \tau)$, resp. According to [3], the operators $K_{\mathbf{k}}^{\pm}(\partial_x, \partial_t)$ will be parametrices for the operators $P_{\mathbf{k}}^{\pm}(\partial_x, \partial_t)$, for $|(\xi, \tau)|$ large, in the sense that $K_{\mathbf{k}}^{\pm} P_{\mathbf{k}}^{\pm} = I + \mathcal{R}_{\mathbf{k}} \sim I$, where I represents the identity operator.

Hence

$$\begin{aligned}
-\Delta - \mathbf{k}\partial_t &= P_{\mathbf{k}} \\
&= P_{\mathbf{k}}(K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-}(I + \mathcal{R}_{\mathbf{k}}) P_{\mathbf{k}}^{-} P_{\mathbf{k}}^{+}) \\
&= P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-} P_{\mathbf{k}}^{-} P_{\mathbf{k}}^{+} + P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-} \mathcal{R}_{\mathbf{k}} P_{\mathbf{k}}^{-} P_{\mathbf{k}}^{+} \\
&= L_{\mathbf{k}} P_{\mathbf{k}}^{-} P_{\mathbf{k}}^{+} + R_{\mathbf{k}},
\end{aligned}$$

where $L_{\mathbf{k}} = P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-}$ and $R_{\mathbf{k}} = P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-} \mathcal{R}_{\mathbf{k}} P_{\mathbf{k}}^{-} P_{\mathbf{k}}^{+}$ is a regularizing operator. Moreover, the symbol of $R_{\mathbf{k}}$ is

$$R_{\mathbf{k}}(\xi, \tau) = \frac{1}{(|\xi| - z_1(\tau))(|\xi| - z_2(\tau))},$$

i.e., the symbol of the operator $R_{\mathbf{k}}$ is the characteristic function associated to the operator $-\Delta - \mathbf{k}\partial_t$.

∎

Time evolution operators

The hypoelliptic operator $-\boldsymbol{\Delta} - \mathbf{k}\partial_{\mathbf{t}}$

We now apply the previous factorization of each $-\Delta - \mathbf{k}\partial_t$ to the study of the linearization of the equation $(-\Delta - \mathbf{k}\partial_t)u = f$. For that, we rewrite this equation as

$$P_{\mathbf{k}}^{+} P_{\mathbf{k}}^{-} u = \tilde{f} - R_{\mathbf{k}} u,$$

where $\tilde{f} = (P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-})^{-1} f$, with $(P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-})^{-1}$ the parametrix of $P_{\mathbf{k}} K_{\mathbf{k}}^{+} K_{\mathbf{k}}^{-}$ and $R_{\mathbf{k}}$ a regularizing Tikhonov-type operator.

The equation $P_{\mathbf{k}}^{-} P_{\mathbf{k}}^{+} u = \tilde{f} - R_{\mathbf{k}} u$ is equivalent to the following system of equations

$$\left\{ \begin{array}{rcl} P_{\mathbf{k}}^{+} u &=& v \\ P_{\mathbf{k}}^{-} v &=& \tilde{f} - R_{\mathbf{k}} u \end{array} \right. , \tag{2.8}$$

and consequently we reduce our equation to a system of first order equations. Introducing the operator

$$Q_{\mathbf{k}}(\partial_x, \partial_t) = \mathbf{k}\partial_t + P_{\mathbf{k}}^{+}(\xi, \partial_t)\partial_x + P_{\mathbf{k}}^{-}(\xi, \partial_t)\partial_x, \tag{2.9}$$

we reduce our previous system to

$$\begin{cases} Q_{\mathbf{k}}(\partial_x, \partial_t)w_1 &= v \\ Q_{\mathbf{k}}(\partial_x, \partial_t)w_2 &= \tilde{f} - R_{\mathbf{k}}u \end{cases}.$$

Letting $w_2 = \partial_x w_1$ we can write (2.9) as a matricial equation

$$(\partial_t - \mathcal{A}_{\mathbf{k}}(t))\mathbf{w} = \mathbf{g}, \tag{2.10}$$

where $\mathbf{w} = (w_1, w_2)^T$, $g = (0, g)^T$ and $\mathcal{A}_{\mathbf{k}}$ is the matrix

$$\begin{bmatrix} 0 & 1 \\ P_{\mathbf{k}}^{-} & P_{k}^{+} \end{bmatrix}. \tag{2.11}$$

$\mathcal{A}_{\mathbf{k}}$ is a matrix valued pseudodifferential operator whose symbol $\sigma(\mathcal{A}_{\mathbf{k}}) = a(\xi, \tau)$ belongs to $S^1_{0,1}$.

We also note that since $\det(\tau I - \sigma(\mathcal{A}_{\mathbf{k}})) = Q_{\mathbf{k}}(\xi, \tau)$, the eigenvalues of $\sigma(\mathcal{A}_{\mathbf{k}})$ are the roots of $Q_{\mathbf{k}}(\xi, \tau)$.

Localization of the eigenvalues of the matrix $\mathcal{A}$

Let K be a compact subset of Ω and

$$N_{\mathbf{k}}(K) = \left\{(\zeta, \tau) \in \mathbb{C}^{m+1} : \ Q_{\mathbf{k}}(\zeta, \tau) = 0\right\},$$

for $(x, t) \in K$. Moreover, for $(\xi, \tau) \in \mathbb{R}^{m+1}$, let $d((\xi, \tau), N_{\mathbf{k}}(K))$ be the distance from (ξ, τ) to $N_{\mathbf{k}}(K)$.

Lemma 2.3.2 *Consider the pseudodifferential operator (2.9). For each compact set $K \subset \Omega$, there exists a constant $C = C(K) > 0$ such that*

$$C^{-1} \leq d \sum_{j=1}^{2} \left(\frac{|\partial_{\xi_j} Q_{\mathbf{k}}(\xi, \tau)|}{|Q_{\mathbf{k}}(\xi, \tau)|} \right)^{\frac{1}{j}} \leq C, \tag{2.12}$$

for $d := d((\xi, \tau), N_{\mathbf{k}}(K))$, $(\xi, \tau) \in \mathbb{R}^{m+1}$, $(x, t) \in K$ and $Q_{\mathbf{k}}(\xi, \tau) \neq 0$.

The proof of this result follows the same steps as in the proof of the Lemma 4.1 in [3]. The main difference is that, while in this lemma we deal with partial differential operators and prove the inequality (2.12) (where the derivatives of Q are taken with respect to all the variables (ξ,τ)), in our case we are dealing with the $\mathbf{k}-$operator, which is a pseudodifferential operator.

Theorem 2.3.3 *For each compact $K \subset \Omega$, there exists positive constants $M(K)$, C_1, C_2 such that whenever $|\tau| > M$, the set of zeros, $\xi(\tau)$, of $Q_{\mathbf{k}}(\xi,\tau)$ for $(x,t) \in K$ is contained in the subset of the complex plane defined by*

$$|\xi| \leq C_1(1+|\tau|), \qquad |\mathrm{Im}(\xi)| \geq C_2|\tau|. \tag{2.13}$$

Proof: Initially we have the following inequality

$$|\xi| \quad \leq \quad 1+\max\{|P^-_{\mathbf{k}}(\xi,\tau)|,\ |P^+_{\mathbf{k}}(\xi,\tau)|\}. \tag{2.14}$$

Since $P^{\pm}_{\mathbf{k}}(\xi,\tau)$ belongs to $S^1_{1,0}$, we obtain the first inequality of our result. It follows from (H1) and (2.12) that for each compact set K there is a constant $C = C(K) > 0$ such that for $|\tau| > M(K)$

$$d \geq C(1+|\tau|). \tag{2.15}$$

If $(\zeta,\tau) \in N_{\mathbf{k}}(K)$, then $d(\mathrm{Re}(\zeta,\tau), N_{\mathbf{k}}(K)) \leq |\mathrm{Im}(\zeta,\tau)|$.

It follows from (2.15) that

$$|Re(\zeta)| \leq C|\mathrm{Im}(\zeta,\tau)|.$$

Hence for $|\tau| > M(K)$ and $(\xi,\tau) \in N_{\mathbf{k}}(K)$

$$|\tau| \leq C|\mathrm{Im}\xi|, \tag{2.16}$$

which is our second inequality.

■

Parametrix of $-\Delta - \mathbf{k}\partial_t$

Taking into account the definition of parametrix for a hypoelliptic operator, we can say that for fixed t' such that $0 \leq t' < T$ a pseudodifferential operator

$$U_{\mathbf{k}}(t,t') : \mathcal{E}'(\Omega, \mathbb{C}^2) \to \mathcal{D}'(\underline{\Omega}, \mathbb{C}^2)$$

depending smoothly on $t \in [t', T)$ is the parametrix for the operator $\mathbf{k}\partial_t - \mathcal{A}_{\mathbf{k}}(t)$, if

$$\begin{cases} \mathbf{k}\dfrac{dU_{\mathbf{k}}(t,t')}{dt} - \mathcal{A}_{\mathbf{k}}(t) \circ U_{\mathbf{k}}(t,t') \sim 0 & \text{in} \quad \Omega \\ \\ U_{\mathbf{k}}(t,t')|_{t=t'} \sim I & \text{in} \quad \underline{\Omega} \end{cases} . \tag{2.17}$$

We note that $U_{\mathbf{k}}(t,t')$ is defined modulo regularizing operators on $\underline{\Omega}$. For our case we can prove the existence of the parametrix as follows.

The operator $U_{\mathbf{k}}(t,t')$ is defined by

$$U_{\mathbf{k}}(t,t')u = (2\pi)^{-m} \int e^{ix\xi} \mathcal{U}_{\mathbf{k}}(t,t')\hat{u}(\xi)d\xi, \tag{2.18}$$

for all $u \in C_c^\infty(\underline{\Omega})$, where $\mathcal{U}_{\mathbf{k}}(t,t')$ is the symbol of $U_{\mathbf{k}}(t,t')$. We construct a formal symbol

$$\mathcal{U}_{\mathbf{k}}(t,t') = \sum_{j=0}^{\infty} (\mathcal{U}_{\mathbf{k}})_j(t,t')$$

from which a true symbol can be constructed by use of cut-off functions in the standard way. Proceeding formally, we write

$$(\mathbf{k}\partial_t - \mathcal{A}_{\mathbf{k}}(t))U_{\mathbf{k}}(t,t')u = (2\pi)^{-m} \int e^{ix\xi} (\mathbf{k}\partial_t - a(\partial_x + \xi, \tau))\mathcal{U}_{\mathbf{k}}(t,t')\hat{u}(\xi)d\xi,$$

and we require for each $0 \leq t < T$ that

$$(\mathbf{k}\partial_t - a(\partial_x + \xi, \tau))\mathcal{U}_{\mathbf{k}}(t,t') = 0 \tag{2.19}$$

and $\mathcal{U}_{\mathbf{k}}(t,t') = I$ (identity matrix).

Let $\lambda(\tau) = (1 + |\tau|)$, and consider the expression

$$zI - \lambda^{-1}a(\tau) = \lambda^{-1}(z\lambda I - a(\tau)).$$

It follows from Theorem 2.3.3 that for each compact set $K \subset \Omega$ there exists a positive constants M, C_1, C_2 such that if $(x,t) \in K$ and $|\tau| \geq M$, the eigenvalues of the matrix $\lambda^{-1}a(\xi,\tau)$ lie in $\mathbb{C}^+$ inside the circle

$$|z| \;\; \leq \;\; C_1(1+|\tau|),$$

and in the half plane-plane $Imz \geq C_2$. For any $R \leq M$ and $R \leq |\tau| \leq R+1$, let Γ_R be a contour in the upper half-plane that encircles the eigenvalues of the matrix $\lambda^{-1}a(\tau)$ for $(x,t) \in K$. In view of the previous remarks we could take the length of Γ_R to be less than $2\pi(R+2)$. We are going to represent $\mathcal{U}$ as

$$\mathcal{U}_{\mathbf{k}}(t,t') = \frac{1}{2\pi i}\oint_{\Gamma_R} e^{i\lambda(t-t')z}k(\tau;z)\;dz,$$

where k is a suitable formal symbol $\sum_{j=1}^{\infty} k_j$.

Since $k(\tau;z)$ is going to be a holomorphic function of z, it follows that $\mathcal{U}_{\mathbf{k}}$ remains the same if the contour Γ_R is changed but still encircles the eigenvalues.

To finalize, we want to estimate the symbols

$$(\mathcal{U}_{\mathbf{k}})_j(t,t') = \frac{1}{2\pi i}\oint_{\Gamma_R} e^{i\lambda(t-t')z}k_j(\tau;z)\;dz. \tag{2.20}$$

Theorem 2.3.4 *To every $K \subset \Omega$, there is a constant $c > 0$ such that to every pair of n-tuples $\alpha = (\alpha_1,\ldots,\alpha_n)$, $\beta = (\beta_1,...,\beta_n) \in \mathbb{N}^n$ and to every pair of integers r and N, there exists a constant $C_1 = C_1(\alpha,\beta,r,K)$ such that*

$$|\partial_x^\beta\partial_\xi^\alpha\partial_t^r(\mathcal{U}_{\mathbf{k}})_j(t,t')| \leq C_1(t-t')^{-N}(1+|\tau|)^{1-|\beta|+r-2N}.$$

for all $(x,t) \in K$ and $|\tau| > c$, where $\partial_x^\beta = \partial_{x_1}^{\beta_1}\ldots\partial_{x_n}^{\beta_n}$ and similarly for ∂_ξ^α .

Proof: For $z \in \Gamma_R$, we have

$$|\partial_\xi^\alpha\partial_t^r(e^{i\lambda(t-t')z})| \leq C(t-t')^{-N}(1+|\tau|)^{-|\alpha|}\lambda^{r-N}. \tag{2.21}$$

Using Leibniz formula we can write $\partial_x^\beta\;\partial_\xi^\alpha\;\partial_t^r(e^{i\lambda(t-t')z}k_j(\tau;z))$ as a linear combination of products of the type $\partial_x^{\beta'}\partial_\xi^{\alpha'}\partial_t^r(k_j)\partial_\xi^{\alpha''}\partial_t^{r''}(e^{i\lambda(t-t')z})$ each of which can be estimated by

$$C(t-t')^{-N}(1+|\tau|)^{1-|\beta'|-|r''|}\lambda^{\alpha''-N} \tag{2.22}$$

Also we have that

$$\lambda^{\alpha''-N} \leq (1+|\tau|)^{r-N}.$$

Combining the previous inequalities we have

$$|\partial_x^\beta \partial_\xi^\alpha \partial_t^r (e^{i\lambda(t-t')z} k_j(\tau)) \leq C(t-t')^{-N}(1+|\tau|)^{1-|\beta|+r-2N},$$

and hence the following estimate for our symbol

$$|\partial_x^\beta \partial_\xi^\alpha \partial_t^r (\mathcal{U}_{\mathbf{k}})_j(t,t')| \leq C(t-t')^{-N}(1+|\tau|)^{1-|\beta|+r-2N} \oint_{\Gamma_R} |dz|.$$

Since $C \oint_{\Gamma_R} |dz| \leq C(2\pi(R+2)) = C_1$ we finally obtain

$$|\partial_x^\beta \partial_\xi^\alpha \partial_t^r (\mathcal{U}_{\mathbf{k}})_j(t,t')| \quad \leq \quad C_1(t-t')^{-N}(1+|\tau|)^{1-|\beta|+r-2N}.$$

■

The particular case of the linear $-\Delta - \mathbf{k}\partial_t$ problem

In this section we aim to solve the problem (2.23) by means of hypoelliptic theory. Consider the following initial value problem

$$\left\{ \begin{array}{rl} (-\Delta - \mathbf{k}\partial_t)u(x,t) = f(x,t) & \text{in} \quad \Omega \\ u(x,0) = h(x) & \text{in} \quad \underline{\Omega} \end{array} \right. , \tag{2.23}$$

where $f \in C^\infty(\Omega)$ and $h \in C^\infty(\underline{\Omega})$. By Definition 2.3 in page 25 of [4] we have that Problem (2.23) is hypoelliptic.

To solve Problem (2.23) it is sufficient to study the homogeneous problem

$$\left\{ \begin{array}{rl} (-\Delta - \mathbf{k}\partial_t)u(x,t) = 0 & \text{in} \quad \Omega \\ u(x,0) = h(x) & \text{in} \quad \underline{\Omega} \end{array} \right. . \tag{2.24}$$

If u_1 is any solution of $(-\Delta - \mathbf{k}\partial_t)u = f$ and u_2 is a solution of the homogeneous problem (2.24) with h substituted for $h - u_1$, then $u = u_1 + u_2$ satisfies (2.23). In view of (2.7) this is equivalent modulo a Tikhonov operator to solve the problem

$$\left\{ \begin{array}{ll} P_{\mathbf{k}}^{+} u(x,t) = 0 & \text{in} \quad \Omega \\ u(x,0) = h(x) & \text{in} \quad \underline{\Omega} \end{array} \right. . \tag{2.25}$$

Since we had constructed the parametrix of the operator $-\Delta - \mathbf{k}\partial_t$ in (2.18), we have that the solution u of (2.25) is equal to $U_{\mathbf{k}}h$.

In one hand, taking into account [4], we can guarantee that the solution obtained previously for the $-\Delta - \mathbf{k}\partial_t-$problem is unique. In the other hand, from the ideas presented in [17] we conclude that the unique solution of the $-\Delta - \mathbf{k}\partial_t$ problem converges, when $\epsilon \to 0$, to the unique solution of the classical problem. Combining this two facts we can ensure that $U_{\mathbf{k}}h$ converges, when $\epsilon \to 0$, to the solution of the following problem

$$\begin{cases} (-\Delta - i\partial_t)u(x,t) = 0 & \text{in} \quad \Omega \\ u(x,0) = h(x) & \text{in} \quad \underline{\Omega} \end{cases},$$

where $\Omega = \underline{\Omega} \times [0,T) \subset \mathbb{R}^n \times \mathbb{R}_0^+$, $f \in C^\infty(\Omega)$ and $h \in C^\infty(\underline{\Omega})$.

Chapter 3

Continuous calculus operator

"I am so happy to have escaped to the terrible mechanics...which I never understood. Now everything is linear, everything can be superposed."

Erwin Schrödinger

It is well-know that methods of complex function theory are powerful tools to solve elliptic boundary value problems in the plane. Most of the advantage of the complex theory are preserved when we use Clifford algebras. From 80's on, second order elliptic boundary value problems were investigated systematically in a self contained theory. Questions of existence, uniqueness and regularity were included in this theory and convenient representations of the solutions were obtained. These integral representation formulas are adapted to the following necessary numerical evaluation of the solutions. In [39] and [47] the authors study several of applications to the quaternions case.

The main purpose of this chapter is to adapt these methods of Clifford analysis to the study of second order time-dependent operators in higher dimensions, with particular emphasis to the Schrödinger equation. With the regularization procedure indicated previously, we obtain existence and uniqueness results for the linear Schrödinger problem with zero-boundary conditions and an explicit expression for this solution. Opposite to the methods of the previous chapter, this solution can be implemented into a stable numerical algorithm. In the the next chapter we will apply this method to the cubic NLS problem, by first developing the necessary theoretical results that we then implement numerically.

The chapter is structured as follows: first we present a convenient factorization of the second order time dependent operators $-\Delta \pm \alpha\partial_t$ in terms of the first order operators $D_\pm := D + \mathfrak{f}\partial_t \pm \alpha\mathfrak{f}^\dagger$. For the homogeneous operator associated to $D_\pm$ we construct, in Subsection 3.1.2, a proper Fischer decomposition. In the second section we apply a regularization to the non-stationary Schödinger operator. We study the arising associated integral operators and apply its properties to generalize some classical results for our regularized case, for example, the Cauchy's integral formula, the Mean-value formula, etc., to obtain a proper decomposition of the L_p-space in terms of the kernel of the operator $D+\mathfrak{f}\partial_t - i\mathfrak{f}^\dagger$, and to present an application to the resolution of linear Schrödinger problem with zero-boundary data.

3.1 Time-dependent operators

Here we develop a function theory for time-dependent operators. One possible approach is to consider the square root of the Laplace operator for studying its solutions, but this will force us to use fractional derivatives and symbol calculus, which are not easy to handle in the numerical part. To avoid this problem we use the idea proposed in [19], which consists in embedding the vector space $\mathbb{R}^n$ in $\mathbb{R}^{1,n+1}$ by introducing two additional basis elements (a Witt basis) which we can use to factorize time-dependent operators acting in the original space $\mathbb{R}^n$.

3.1.1 Factorization of time-dependent operators

Consider the operator $-\Delta - \alpha\partial_t$. When $\alpha = -1$ we have the classical heat operator and when $\alpha = -\dfrac{2mi}{\hbar}$ we have the classical Schrödinger operator. For simplification of the future work we will consider the cases $\alpha = \pm 1$ and $\alpha = \pm i$ for the forward/backward heat and Schrödinger operators, respectively. While the forward (classic) heat equation allows us to calculate the temperature distribution for a future time based on the current (or starting) temperature distribution, the backward heat equation corresponds to the case of calculating a past temperature distribution. The fact of calculating a past distribution can be modeled by a negative thermal conduction coefficient. This leads to the backward heat equation. As it was indicated previously, we will consider $\mathbb{R}^{0,n}$ as a subspace of $\mathbb{R}^{1,n+1}$. For that purpose, we add two new basis elements e_+ and e_+ such that

$$e_+^2 = +1 \qquad e_-^2 = -1$$

$$e_+ e_j + e_j e_+ = 0, \quad e_- e_j + e_j e_- = 0, \quad j = 1, \cdots, n.$$

Since we want to study time-dependent problems, we can consider the square root of $-\Delta \pm \alpha \partial_t$ inside the Clifford algebra, but in consequence we will deal with fractional derivatives.

To solve the problem of fractional derivatives, we can use the elements e_+ and e_- to construct new elements $\mathfrak{f} = \dfrac{e_+ - e_-}{2}$ and $\mathfrak{f}^\dagger = -\dfrac{e_+ + e_-}{2}$, such that

$$(\mathfrak{f})^2 = (\mathfrak{f}^+)^2 = 0 \qquad \mathfrak{f}\mathfrak{f}^+ + \mathfrak{f}^+\mathfrak{f} = 1$$

$$\mathfrak{f} e_j + e_j \mathfrak{f} = \mathfrak{f}^+ e_j + e_j \mathfrak{f}^+ = 0.$$

The set $\{\mathfrak{f}, \mathfrak{f}^\dagger\}$ is said to be a Witt basis for $\mathbb{R}^{1,1}$. This construction allows us to define a suitable factorization of our time-dependent operators, where only partial derivatives are used.

Therefore, a $\mathbb{R}_{1,n+1}-$ valued polynomial function $u = u(x,t)$ can be decomposed as

$$\begin{aligned} u(x,t) &= u_1(x,t) + \mathfrak{f} u_2(x,t) + \mathfrak{f}^+ u_3(x,t) + \mathfrak{f}\mathfrak{f}^+ u_4(x,t) \\ &= u_1 + \mathfrak{f} u_2 + \mathfrak{f}^+ u_3 + \mathfrak{f}\mathfrak{f}^+ u_4, \end{aligned} \tag{3.1}$$

where the components u_i, $i = 1, 2, 3, 4$, are the $\mathbb{R}_{0,n}-$valued polynomials, i.e.,

$$u_i(x,t) = \sum_A p_{i,A}(x,t) e_A,$$

where $p_{i,A}(x,t)$ are real valued polynomials.

With this previous construction and considering $\Omega \subset \mathbb{R}^n \times \mathbb{R}_0^+$, a bounded domain with a piecewise smooth boundary $\Gamma = \partial\Omega$, we can introduce the following definition

Definition 3.1.1 *For a function $u \in W_p^1(\Omega)$, with $1 \le p < +\infty$, we define the forward/backward parabolic-type Dirac operator as*

$$D_\pm u = (D + \mathfrak{f}\partial_t \pm \alpha \mathfrak{f}^\dagger) u, \tag{3.2}$$

where D stands for the (spatial) Dirac operator.

Taking into account the definition of homogeneous operator presented in Section 18.2 of [42] we define, in connection to the previous operators, the homogeneous operator

$$D_* u = (D + \mathfrak{f}\partial_t)u. \tag{3.3}$$

By the multiplication rules defined for the elements of the Witt basis, it is immediate that these operators are such that

$$(D_\pm)^2 u = (-\Delta \pm \alpha\partial_t)u,$$
$$(D_*)^2 u = -\Delta u.$$

Taking into account the homogeneity properties of the operator D_*, we will study, in the next section, the existence of a Fischer decomposition for the case of the heat operator. Since the operator $D_\pm$ is not homogeneous, we are not able to construct a Fischer decomposition using this operator.

3.1.2 Fischer decomposition for the homogeneous operator $\mathbf{D}_*$

Now we will study the existence of the Fischer decomposition for the case of the heat operator, i.e., when we consider $\alpha = 1$ in the operators (3.2). In order to do that, we need to introduce the following definition

Definition 3.1.2 *For $k \in \mathbb{N}_0$ and arbitrary $R,\ S \in \mathcal{P}(k;\mathbb{R}_{1,n+1})$, where $\mathcal{P}(k;\mathbb{R}_{1,n+1})$ is the space of $\mathbb{R}_{1,n+1}$homogeneous polynomials of degree k, we define the Fischer inner product for the parabolic case as*

$$< R, S >_k = [\overline{R(D,\partial_t)}S\Big|_{(x,t)=(0,0)}]_0 = \sum_{|\alpha|=k} \alpha![\overline{a_\alpha} b_\alpha]_0, \tag{3.4}$$

where $a_\alpha, b_\alpha \in \mathbb{C}\setminus\mathbb{R}$ are the coefficients of R and S, and $\overline{R(D,\partial_t)}$ is the differential operator obtained in a similar procedure as in the classic case (c.f. [22]).

Since $\overline{\mathfrak{f}} = -\mathfrak{f}$, $\overline{\mathfrak{f}^\dagger} = -\mathfrak{f}^\dagger$, we get

$$\begin{aligned} < (x - t\mathfrak{f})R, S >_k &= < xR, S >_k - < t\mathfrak{f}R, S >_k \\ &= -\langle R, DS\rangle_{k-1} - [\overline{\partial_t \mathfrak{f} R(D, \partial_t)} S\Big|_{(x,t)=(0,0)}]_0 \\ &= -\langle R, DS\rangle_{k-1} - [\overline{R(D, \partial_t)}\ \mathfrak{f}\partial_t S\Big|_{(x,t)=(0,0)}]_0 \\ &= -\langle R, (D + \mathfrak{f}\partial_t)S\rangle_{k-1}. \end{aligned}$$

Hence, we get the following lemma

Lemma 3.1.3 *For every $k \in \mathbb{N}$, and arbitrary $R \in \mathcal{P}(k-1; \mathbb{R}_{1,n+1})$ and $S \in \mathcal{P}(k; \mathbb{R}_{1,n+1})$ we have*

$$\langle (x - t\mathfrak{f})R, S\rangle_k = -\langle R, (D + \mathfrak{f}\partial_t)S\rangle_{k-1}. \tag{3.5}$$

This result express the connection between the decomposition of the space of homogeneous polynomial solutions of the operator (3.3) and the variable $(x - t\mathfrak{f}^\dagger)$. One has

Theorem 3.1.4 *The space $\mathcal{P}(k; \mathbb{R}_{1,n+1})$ admits the following decomposition*

$$\mathcal{P}(k; \mathbb{R}_{1,n+1}) = \mathbb{M}^+(k; \mathbb{R}_{1,n+1}) \oplus^\perp (x - t\mathfrak{f}^\dagger)\mathcal{P}(k-1; \mathbb{R}_{1,n+1})l \tag{3.6}$$

$$= \sum_{s=0}^{k} \oplus^\perp (x - t\mathfrak{f}^\dagger)^s \mathbb{M}^+(k - s; \mathbb{R}_{1,n+1}), \tag{3.7}$$

where $\mathbb{M}^+(k, \mathbb{R}_{1,n+1})$ denotes the space of homogeneous polynomials of degree k which are null-solutions of the homogeneous operator (3.3).

The proof of this result is based on the ideias presented in [22], page 206. The equality (3.7) is a corollary of (3.6). To prove (3.6) it is sufficient to prove that $\mathbb{M}^+(k; \mathbb{R}_{1,n+1}) = ((x - t\mathfrak{f}^\dagger)\mathcal{P}(k-1; \mathbb{R}_{1,n+1}))^\perp$.

3.1.3 Powers of D_*

We now use the previous conclusions to study the powers of the homogeneous operator D_*. Taking into account the relation (3.5) and

$$(x - t\mathfrak{f}^\dagger)^s = \begin{cases} (-1)^n |x|^{2m} & \text{for } s = 2m, \\ (-1)^n (x - t\mathfrak{f}^\dagger)|x|^{2m} & \text{for } s = 2m+1, \end{cases} \tag{3.8}$$

we can write every $u \in \mathcal{P}(k;\mathbb{R}_{1,n+1})$ as

$$\begin{aligned} u(x,t) &= u_k(x,t) + (x-\mathfrak{f}^\dagger t)u_{k-1}(x,t) - |x|^2 u_{k-2}(x,t) \\ &\quad - (x-\mathfrak{f}^\dagger t)|x|^2 u_{k-3}(x,t) + \cdots + (x-\mathfrak{f}^\dagger t)^k u_0(x,t) \end{aligned} \tag{3.9}$$

where $u_s = u_s^{[0]} + \mathfrak{f}u_s^{[1]} + \mathfrak{f}^\dagger u_s^{[2]} + \mathfrak{f}\mathfrak{f}^\dagger u_s^{[3]}$, $(s = 0,...,k\ )$. We establish the following result

Lemma 3.1.5 *The components* $u_s = u_s^{[0]} + \mathfrak{f}u_s^{[1]} + \mathfrak{f}^\dagger u_s^{[2]} + \mathfrak{f}\mathfrak{f}^\dagger u_s^{[3]}$, *with* $s = 0,...,k$, *are in* $\mathbb{M}^+(k;\mathbb{R}_{1,n+1})$ *if and only if they satisfy the system:*

$$\begin{cases} Du_s^{[0]} = Du_s^{[2]} = 0 \\ Du_s^{[1]} = \partial_t u_s^{[0]} \\ Du_s^{[3]} = -\partial_t u_s^{[2]}. \end{cases} \tag{3.10}$$

Proof: The components $u_s = u_s^{[0]} + \mathfrak{f}u_s^{[1]} + \mathfrak{f}^\dagger u_s^{[2]} + \mathfrak{f}\mathfrak{f}^\dagger u_s^{[3]}$, $(s = 0,...,k)$, are in $\mathbb{M}^\perp(k;\mathbb{R}_{1,n+1})$ if and only if

$$\begin{aligned} 0 &= (D+\mathfrak{f}\partial_t)(u_s^{[0]} + \mathfrak{f}u_s^{[1]} + \mathfrak{f}^\dagger u_s^{[2]} + \mathfrak{f}\mathfrak{f}^\dagger u_s^{[3]}) \\ &= Du_s^{[0]} + \mathfrak{f}(\partial_t u_s^{[0]} - Du_s^{[1]}) - \mathfrak{f}^\dagger Du_s^{[2]} + \mathfrak{f}\mathfrak{f}^\dagger(\partial_t u_s^{[2]} + Du_s^{[3]}). \end{aligned}$$

From the previous equality we obtain the system needed.

■

Given $u \in \mathcal{P}(k;\mathbb{R}_{1,n+1})$, we want to obtain sufficient conditions such that u belongs to the kernel of the operator $(D_*)^{k+1}$, i.e.

$$(D+\mathfrak{f}\partial_t)^{k+1}u(x,t) = 0. \tag{3.11}$$

To obtain the solutions of (3.11), is sufficient to solve the following system of equations

$$(D+\mathfrak{f}\partial_t)^{s+1}((x-t\mathfrak{f}^\dagger)^s u_{k-s}(x,t)) = 0, \qquad s = 0,1,\cdots,k \tag{3.12}$$

with each $u_{k-s} \in \mathbb{M}^+(k-s;\mathbb{R}_{1,n+1})$.

Taking into account (3.8) we obtain two different classes of equations:

- Case of $s = 2m$ even

$$(D+\mathfrak{f}\partial_t)\Delta_x^m\ (|x|^{2m}u_{k-2m}(x,t)) = 0, \tag{3.13}$$

- Case of $s = 2m + 1$ odd

$$\Delta_x^{m+1} \left(|x|^{2m}(x - t\mathfrak{f}^\dagger)u_{k-2m-1}(x,t)\right) = 0, \tag{3.14}$$

where Δ_x denotes the Laplacian in the space variable x.

The difference between the even and the odd case suggest the splitting of each $u_s \in \mathbb{M}^+(s; \mathbb{R}_{1,n+1})$ in similar way as in (3.1), but now in terms of the Witt basis elements. Therefore, we have in the case of $s = 2m$ that

$$\begin{aligned} u_{k-2m} &= \tilde{u}^{[0]}_{k-2m} + \mathfrak{f}\tilde{u}^{[1]}_{k-2m} + \mathfrak{f}^\dagger\tilde{u}^{[2]}_{k-2m} + \mathfrak{f}\mathfrak{f}^\dagger\tilde{u}^{[3]}_{k-2m} \\ &= (\tilde{u}^{[0]}_{k-2m} + \mathfrak{f}^\dagger\tilde{u}^{[2]}_{k-2m}) + \mathfrak{f}(\tilde{u}^{[1]}_{k-2m} + \mathfrak{f}^\dagger\tilde{u}^{[3]}_{k-2m}) \\ &= u^{[0]}_{k-2m} + \mathfrak{f}u^{[1]}_{k-2m}, \end{aligned} \tag{3.15}$$

where each $u^{[i]}_{k-2m}$ is $(\mathbb{R}_{0,n} + \mathfrak{f}^\dagger\mathbb{R}_{0,n})$-valued, for $i = 0, 1$. For $s = 2m + 1$ we have that

$$u_{k-2m-1} = u^{[1]}_{k-2m-1} + \mathfrak{f}^\dagger u^{[2]}_{k-2m-1}, \tag{3.16}$$

where $u^{[i]}_{k-2m-1}$ is $(\mathbb{R}_{0,n} + \mathfrak{f}\mathbb{R}_{0,n})$-valued, for $i = 0, 1$.

From equation (3.13) we obtain that the functions u_{k-2n} must verify one of the following conditions

1. The function $|x|^{2m}u^{[0]}_{k-2m}(x,t)$ is a $l-$harmonic function for one $l \in \{1, ..., m\}$ and $|x|^{2m}u^{[1]}_{k-2m}(x,t)$ is $j-$harmonic for one $j \in \{1, ..., m\}$.

2. There exists $l, j \in \{0, ..., m\}$ such that

$$\begin{cases} \Delta^l D(|x|^{2m}u^{[0]}_{k-2m}(x,t)) = 0 \\ \Delta^j D(|x|^{2m}u^{[1]}_{k-2m}(x,t)) = \Delta^j(|x|^{2m}\partial_t u^{[0]}_{k-2m}(x,t)). \end{cases}$$

The last condition arises from (3.15) and the equality

$$\begin{aligned} &(D + \mathfrak{f}\partial_t)(|x|^{2m}[u^{[0]}_{k-2m} + \mathfrak{f}u^{[1]}_{k-2m}]) \\ &= D(|x|^{2m}u^{[0]}_{k-2m}) + \mathfrak{f}(|x|^{2m}\partial_t u^{[0]}_{k-2m} - D(|x|^{2m}u^{[1]}_{k-2m})). \end{aligned}$$

For the odd case we obtain from (3.16)

$$\begin{aligned} &(x - t\mathfrak{f}^\dagger)(u^{[0]}_{k-2m-1} + \mathfrak{f}^\dagger u^{[1]}_{k-2m-1}) \\ &= xu^{[0]}_{k-2m-1}(x,t) - \mathfrak{f}^\dagger(tu^{[0]}_{k-2m-1}(x,t) + xu^{[1]}_{k-2m-1}(x,t)) \end{aligned}$$

so that equation (3.11) is satisfied if and only if there exists $l, j \in \{1, ..., m+1\}$ such that

$$\begin{cases} \Delta^l(|x|^{2m} x u^{[0]}_{k-2m-1}(x,t)) = 0 \\ \Delta^j(|x|^{2m}(t u^{[0]}_{k-2m-1}(x,t) + x\partial_t u^{[1]}_{k-2m-1}(x,t))) = 0. \end{cases}$$

Example 3.1.6 *A simple example of a polynomial function u of degree k, which is a solution of the equation (3.12) is*

$$\begin{aligned} u(x,t) \quad = \quad & \sum_{i=0}^{k} (-1)^k \, S_{2k}(x,t) + \mathfrak{f} \sum_{i=0}^{k} \tilde{S}_{2k}(x,t) + \\ & \sum_{i=0}^{k} \hat{S}_{2k+1}(x,t) - \mathfrak{f}^{\dagger} t x^{-1} \sum_{i=1}^{k} (x^{2k}+1) \hat{S}_{2k-1}(x,t), \end{aligned}$$

where the functions $S_{2k}(x,t)$, $\tilde{S}_{2k}(x,t)$, $\hat{S}_{2k+1}(x,t)$, $\hat{S}_{2k-1}(x,t)$, are spherical monogenic in the x variable. Taking into account that a finite sum of monogenic functions is a monogenic function, we can redescribe u as

$$u(x,t) \quad = \quad W(x,t) + \mathfrak{f}\tilde{W}(x,t) + \hat{W}(x,t) - \mathfrak{f}^{\dagger} t x^{-1} \hat{W}(x,t),$$

where the functions $W(x,t)$, $\tilde{W}(x,t)$, $\hat{W}(x,t)$ are spherical monogenics in the x variable.

The function u admits a decomposition similar to (3.9). In this case we can say that the components of the functions $u_{k-i}(x,t)$, with $i = 0, ..., k$, verify the conditions

- *If $k-i$ is even then*

$$u^{[0]}_{k-i}(x,t) = |x|^{-(k-i)} S(x,t) \qquad u^{[1]}_{k-i} = |x|^{-(k-i)} \tilde{S}(x,t),$$

  where the functions $S(x,t)$ and $\tilde{S}(x,t)$ are spherical monogenic in the x variable.

- *If $k-i$ is odd then*

$$u^{[0]}_{k-i}(x,t) = |x|^{-(k-i)} S(x,t) \qquad u^{[1]}_{k-i}(x,t) = t S(x,t),$$

  where the function $S(x,t)$ is again a spherical monogenic in the x variable.

3.2 Operator calculus for the Schrödinger operator

We now concentrate our efforts in the Schrödinger operator, i.e., we will consider $\alpha = i$ in (3.2). Let us start with the construction of the fundamental solution for the backward Schrödinger operator $-\Delta + i\partial_t$. For that purpose, we consider the fundamental solution of the heat operator

$$e(x,t) = \frac{H(t)}{(4\pi t)^{\frac{n}{2}}} \exp\left(-\frac{|x|^2}{4t}\right), \tag{3.17}$$

where $H(t)$ denotes the Heaviside function. Let us remark that the previous fundamental solution verifies

$$(-\Delta + \partial_t)e(x,t) = \delta(x)\delta(t).$$

We apply to (3.17) the Wick rotation $t \to it$. There we obtain

$$(-\Delta + i\partial_t)e(x,it) = -\Delta e(x,it) - \partial_{it} e(x,it) = \delta(x)\delta(it) = -i\delta(x)\delta(t),$$

i.e., the fundamental solution for the Schrödinger operator $-\Delta + i\partial_t$ is

$$\begin{aligned} e_+(x,t) &= ie(x,it) \\ &= i\ \frac{H(t)}{(4\pi it)^{\frac{n}{2}}} \exp\left(-i\ \frac{|x|^2}{4t}\right). \end{aligned} \tag{3.18}$$

Then we have

Definition 3.2.1 *Given the fundamental solution $e_+ = e_+(x,t)$ we have as fundamental solution $E_+ = E_+(x,t)$ for the parabolic-type Dirac operator D_+ the function*

$$\begin{aligned} E_+(x,t) &= e_+(x,t)D_+ \\ &= i\frac{H(t)}{(4\pi it)^{\frac{n}{2}}} \exp\left(\frac{-i|x|^2}{4t}\right)\left(-i\frac{x}{2t} + \mathfrak{f}\left(\frac{i|x|^2}{4t^2} + \frac{n}{2t}\right) + i\mathfrak{f}^\dagger\right). \end{aligned} \tag{3.19}$$

3.2.1 Regularization of the fundamental solution

Any fundamental solution e_+ for the Schrödinger operator has singularities in the hyperplane $t = 0$. This produces a dramatic difference from the classical 1-point singularity for the hypoelliptic operators in so far as they are non-removable. This carries additional problems for the study of the Teodorescu and Cauchy-Bitsadze operators, where we no longer have the convergence, in the classical sense, of the integrals that define those operators.

The process of regularization (see [64]) creates a family of operators and correspondent fundamental solutions, which are locally integrable in $\mathbb{R}^n \times \mathbb{R}_0^+ \setminus \{(0,0)\}$. We prove that these family converge to the original operator and fundamental solutions, respectively, when $\epsilon \to 0$.

To this end, we apply the modified Wick rotation $t \to (\epsilon + i)t$ to the heat operator

$$(-\Delta + \mathbf{k}\partial_t)[(\epsilon + i)e(x, (\epsilon + i)t)] = \delta(x)\delta(t), \tag{3.20}$$

with $\mathbf{k} = \frac{\epsilon+i}{\epsilon^2+1}$. Let us remark that, for each $\epsilon > 0$, $-\Delta + \mathbf{k}\partial_t$ is a hypoelliptic operator and therefore we ensure the good behavior for the associated integral operators. In addition, we get a family of fundamental solutions for this family of operators given by

$$\begin{aligned} e_+^\epsilon(x,t) &= (\epsilon + i)e(x, (\epsilon + i)t) \\ &= (\epsilon + i)\, \frac{H(t)}{(4\pi(\epsilon + i)t)^{\frac{n}{2}}} \exp\left(-\frac{(\epsilon + i)|x|^2}{4(\epsilon^2 + 1)t} \right), \quad \epsilon > 0. \end{aligned}$$

This leads us to the following regularized parabolic-type Dirac operator.

Definition 3.2.2 *For a function $u \in W_p^a(\Omega)$, with $1 \leq p < +\infty$ and $a \in \mathbb{N}$, we define the forward/backward regularized parabolic-type Dirac operator as*

$$D_\pm^\epsilon u = (D + \mathfrak{f}\partial_t \pm \mathbf{k}\mathfrak{f}^\dagger)u, \tag{3.21}$$

where D stands for the spatial Dirac operator.

This operator factorizes the correspondent forward/backward regularized Schrödinger operator, i.e.,

$$(D_\pm^\epsilon)^2 u = (-\Delta \pm \mathbf{k}\partial_t)u.$$

For this regularized operator we have that $D_\pm^\epsilon : W_p^1(\Omega) \to L_p(\Omega)$, $1 \leq p < +\infty$, and we establish the following result.

Theorem 3.2.3 *For the family of parabolic-type Dirac operators D_+^ϵ, with $\epsilon > 0$, we have the following convergence:*

$$||D_+ u - D_+^\epsilon u||_{L_1(\Omega)} \to 0,$$

where $u \in W_1^1(\Omega)$.

Proof: We have

$$||(D_+ - D_+^\epsilon)u||_{L_1(\Omega)} = \left|\left|\left(i - \frac{\epsilon + i}{\epsilon^2+1}\right)u\right|\right|_{L_1(\Omega)}.$$

In the previous expression, we can say that

$$\lim_{\epsilon\to 0^+}\left(i - \frac{\epsilon+i}{\epsilon^2+1}\right) = 0,$$

which implies our assertion.

■

We now construct the family of regularized fundamental solutions for this first-order operator.

Definition 3.2.4 *Given a fundamental solution $e_+^\epsilon = e_+^\epsilon(x,t)$ of the equation (3.20), we have that the function $E_+^\epsilon(x,t) = D_+^\epsilon e_+^\epsilon(x,t)$ is a fundamental solution of the operator D_+^ϵ.*

Easy calculations (see [17]) give

$$\begin{aligned} E_+^\epsilon(x,t) &= D_+^\epsilon e_+^\epsilon(x,t) \\ &= e_+^\epsilon(x,t)\left[\frac{x}{2(\epsilon+i)t} + \mathfrak{f}\left(\frac{n}{2t} - \frac{|x|^2}{4(\epsilon+i)t^2}\right) + \mathbf{k}\mathfrak{f}^\dagger\right]. \end{aligned} \tag{3.22}$$

The following result shows the regularity of such fundamental solution.

Theorem 3.2.5 *We have that $E_+^\epsilon \in L_p(\Omega)$ for all $1 \le p < +\infty$.*

Proof: Taking into account expression (3.22) for the regularized fundamental solution E_+^ϵ, we have the following inequality

$$\begin{aligned} ||E_+^\epsilon||_{L_p(\Omega)} &= ||D_+^\epsilon e_+^\epsilon||_{L_p(\Omega)} \\ &\le ||A_1||_{L_p(\Omega)} + ||A_2||_{L_p(\Omega)} + ||A_3||_{L_p(\Omega)}, \end{aligned}$$

where

$$\begin{aligned} A_1(x,t) &= e_+^\epsilon(x,t)\,\frac{x}{2(\epsilon+i)t} \\ A_2(x,t) &= e_+^\epsilon(x,t)\,\mathfrak{f}\left(\frac{n}{2t} - \frac{|x|^2}{4(\epsilon+i)t^2}\right) \\ A_3(x,t) &= e_+^\epsilon(x,t)\,\mathbf{k}\mathfrak{f}^\dagger. \end{aligned}$$

As Ω is a bounded space-time domain there exists a, b and T such that $\Omega \subset [-a,b]^n \times [0,T]$. Moreover, the change of variables $w = \dfrac{B(x)}{t}$, $dt = -\dfrac{B(x)}{w^2}\,dw$ carries

$$\int_0^T t^{-\frac{np}{2}-p} \exp\left(-\frac{B(x)}{t}\right) dt = [B(x)]^{1-\frac{np}{2}-p}\,\Gamma\left(\frac{np}{2}+p-1, \frac{B(x)}{T}\right)$$
$$\int_0^T t^{-\frac{np}{2}-2p} \exp\left(-\frac{B(x)}{t}\right) dt = [B(x)]^{1-\frac{np}{2}-2p}\,\Gamma\left(\frac{np}{2}+2p-1, \frac{B(x)}{T}\right)$$

Therefore, for such terms we have the following estimates

$$\begin{aligned}
||A_1||_{L_p(\Omega)} &\leq 2^{\frac{n}{2}} \left(\left(\frac{\epsilon^2+1}{2(4\pi)^{\frac{n}{2}}} \right)^p \int_{[-a,b]^n} |x|^p\, [B(x)]^{1-\frac{np}{2}-p}\,\Gamma\left(\frac{np}{2}+p-1, \frac{B(x)}{T}\right) dx \right)^{\frac{1}{p}}, \\
||A_2||_{L_p(\Omega)} &\leq 2^{\frac{n}{2}} \left(\left(\frac{n(\epsilon^2+1)}{2(4\pi)^{\frac{n}{2}}} \right)^p \int_{[-a,b]^n} [B(x)]^{1-\frac{np}{2}-p}\,\Gamma\left(\frac{np}{2}+p-1, \frac{B(x)}{T}\right) dx \right)^{\frac{1}{p}} \\
&\quad + \left(\left(\frac{\epsilon^2+1}{4(4\pi)^{\frac{n}{2}}} \right)^p \int_{[-a,b]^n} |x|^{2p}\, [B(x)]^{1-\frac{np}{2}-2p}\,\Gamma\left(\frac{np}{2}+2p-1, \frac{B(x)}{T}\right) dx \right)^{\frac{1}{p}} \\
||A_3||_{L_p(\Omega)} &\leq 2^{\frac{n}{2}} \left(\left(\frac{\epsilon^2+1}{(4\pi)^{\frac{n}{2}}} \right)^p \int_{[-a,b]^n} \int_0^T \exp\left(-\frac{B(x)}{t}\right) dt dx \right)^{\frac{1}{p}},
\end{aligned}$$

where

$$B(x) = \frac{\epsilon p |x|^2}{4(\epsilon^2+1)}.$$

Taking into account the properties of the incomplete Gamma function we get that the norms $||A_1||_{L_p(\Omega)}$ and $||A_2||_{L_p(\Omega)}$ are bounded. Finally, since $||A_3||_{L_p(\Omega)}$ is expressed by an integral of a Gaussian, it is also bounded for all $\epsilon > 0$. Hence, the norm $||E_-^\epsilon||_{L_p(\Omega)}$ is finite.

■

Moreover, for each $\epsilon > 0$, we have the E_+^ϵ is a regular distribution. We now present a result regarding the convergence in distributional sense of the family of fundamental solutions.

Theorem 3.2.6 *The family of regular distributions E_+^ϵ, with $\epsilon > 0$, converges to E_+ in $W_p^{-\frac{n}{2}+1}(\Omega)$, with $1 \leq p < +\infty$.*

Proof: By the previous theorem we can say that, for every $\epsilon > 0$, E_+^ϵ is a family of locally integrable functions in the compact domain $\Omega \subset [-a,b]^n \times [0,T] \subset \mathbb{R}^n \times \mathbb{R}_0^+$. As $\epsilon \to 0$ we have a pointwise convergence almost everywhere to E_+. Moreover, we can guarantee that there exists a positive constant M, such that $||E_+^\epsilon||_{L_p(\Omega)} \leq M$ for all $1 \leq p < +\infty$ and $\epsilon > 0$. Since $\varphi \in W_p^{\frac{n}{2}-1}(\Omega)$ and $1 \leq p < +\infty$, the product φE_+^ϵ is locally integrable in Ω (see [44]). We have then

$$||\varphi E_+^\epsilon||_{L_p(\Omega)} \leq ||\varphi||_{L_p(\Omega)} ||E_+^\epsilon||_{L_p(\Omega)} \leq ||\varphi||_{L_p(\Omega)} M,$$

thus proving that the elements of the family φE_+^ϵ are dominated by $||\varphi||_{L_p(\Omega)} M$. Applying the Lebesgue theorem

$$\int_\Omega E_+(x,t)\varphi(x,t)\,dxdt = \lim_{\epsilon\to 0^+} \int_\Omega E_+^\epsilon(x,t)\varphi(x,t)\,dxdt \equiv < E_+, \varphi >,$$

we obtain our result.

■

As an immediate consequence of the previous theorem we get the following relation between the distribution defined by E_+^ϵ and E_+.

Theorem 3.2.7 *Given a function $\varphi \in \mathcal{S}'$, we have the following convergence in the distributional sense*

$$\lim_{\epsilon\to 0} \left(E_+^\epsilon * \varphi\right) = \left(E_+ * \varphi\right).$$

Proof: Let us consider $\phi \in \mathcal{D}$. We have

$$\lim_{\epsilon\to 0} (E_+^\epsilon * \varphi) = \lim_{\epsilon\to 0} \left\langle E_+^\epsilon * \varphi,\, \phi \right\rangle = \lim_{\epsilon\to 0} \left\langle E_+^\epsilon,\, \varphi * \phi \right\rangle = \left\langle E_+,\, \varphi * \phi \right\rangle.$$

Let us remark that the last simplification is only valid by the application of the convergence result presented in the previous theorem. By the properties of the convolution between distributions we have finally

$$\left\langle E_+,\, \varphi * \phi \right\rangle = \left\langle E_+ * \varphi,\, \phi \right\rangle.$$

■

3.2.2 Regularized Teodorescu and Cauchy-Bitsadze operators

Now we discuss the operators arising in connection to the previous regularization procedure. These operators will be very important in future sections in the treatment of the Schrödinger equation and in the construction of a decomposition of the L_p-space.

In connection with the regularized parabolic-type Dirac operator D_-^ϵ, we introduce the following regularized Stokes' theorem.

Theorem 3.2.8 *For each $u, v \in W_p^1(\Omega),\ 1 \leq p < +\infty$, it holds*

$$\int_{\partial\Omega} v d\sigma_{x,t} u = \int_\Omega [(vD_+^\epsilon)u + v(D_-^\epsilon u)] dxdt \tag{3.23}$$

where the surface element is given by the contraction of the homogeneous operator D_* with the volume element, i.e., $d\sigma_{x,t} = (D_x + \mathfrak{f}\partial_t)\rfloor dxdt$.

In (3.23) if we replace v by E_+^ϵ we obtain the regularized Borel-Pompeiu formula

$$\begin{aligned}&\int_{\partial\Omega} E_+^\epsilon(x - x_0, t - t_0) d\sigma_{x,t}\, u(x,t)\\ &= u(x_0, t_0) - \int_\Omega E_+^\epsilon(x - x_0, t - t_0)(D_-^\epsilon u)(x,t) dxdt,\ (x_0, t_0) \notin \partial\Omega.\end{aligned} \tag{3.24}$$

Moreover, when $u \in \ker(D_-^\epsilon)$ we get the regularized Cauchy's Integral formula

$$\int_{\partial\Omega} E_+^\epsilon(x - x_0, t - t_0) d\sigma_{x,t}\ u(x,t) = u(x_0, t_0). \tag{3.25}$$

Based on expression (3.24) we have the following definition.

Definition 3.2.9 *Let $u \in L_p(\Omega)$. The regularized Teodorescu operator is defined as*

$$T_-^\epsilon u(x,t) \quad = \quad -\int_\Omega E_+^\epsilon(x - z, t - s) u(z,s) dzds, \qquad (x,t) \notin \partial\Omega. \tag{3.26}$$

From the definition we obtain the following results.

Theorem 3.2.10 *The operator T_-^ϵ is bounded from $L_p(\Omega)$ to $L_p(\Omega)$, with $1 \leq p < +\infty$.*

Proof: Let $u \in L_p(\Omega)$, with $1 \leq p < +\infty$. We have

$$\begin{aligned}||T_-^\epsilon u||_{L_p(\Omega)}^p &= 2^{\frac{nr}{2}} \int_\Omega \left|(T_-^\epsilon u)(x,t)\right|^p dxdt\\ &= 2^{\frac{nr}{2}} \int_\Omega \left|\int_\Omega E_+^\epsilon(x - y, t - s) * u(y,s)\, dyds\right|^p dxdt\\ &\leq 2^{\frac{nr}{2}} \int_\Omega \left[\int_\Omega \left|E_+^\epsilon(x - y, t - s) u(y,s)\right| dyds\right]^p dxdt.\end{aligned} \tag{3.27}$$

By Holder's inequality we have, for $\dfrac{1}{p} + \dfrac{1}{q} = 1$

$$\begin{aligned}(3.27) \quad &\leq \quad 2^{\frac{nr}{2}} \int_\Omega \left[||E_+^\epsilon(x - \cdot, t - \cdot)||_{L_q(\Omega)} ||u||_{L_p(\Omega)}\right]^p dxdt\\ &\leq \quad 2^{\frac{nr}{2}} ||u||_{L_p(\Omega)}^p \int_\Omega ||E_+^\epsilon(x - \cdot, t - \cdot)||_{L_q(\Omega)}^p dxdt.\end{aligned}$$

Taking into account Theorem 3.2.5 and the fact that Ω is bounded, we get

$$2^{\frac{nr}{2}}||u||^p_{L_p(\Omega)}\int_\Omega ||E^\epsilon_+(x-\cdot,t-\cdot)||^p_{L_q(\Omega)}dxdt \leq C\,Vol(\Omega)\,||u||^p_{L_p(\Omega)},$$

which is our result.

■

Our next aim will be study of the boundedness of the derivatives of the regularized Teodorescu operator T^ϵ_-.

Theorem 3.2.11 *Let $u \in L_p(\Omega)$, with $1 < p < +\infty$. We have the derivatives of the regularized Teodorescu operator*

$$\partial_{x_k}(T^\epsilon_- u) : L_p(\Omega) \to L_p(\Omega), \quad k = 1, 2, \cdots, n;$$

$$\partial_t(T^\epsilon_- u) : L_p(\Omega) \to L_p(\Omega).$$

are bounded.

Proof: The proof will be divided in two parts: in the first part we consider the case of a cylindrical domain. By classical methods, we show that the essential part for proving the boundedness of the Teodorescu operator is given by the convolution with the derivatives of the fundamental solution. Then, we prove that these convolution operators are bounded in L_p of the cylindrical domain. Finally, in the second part we extend our result to the case of an arbitrary (time dependent) bounded domain $\Omega \subset \mathbb{R}^n \times \mathbb{R}^+_0$.

First, we consider a cylindrical domain of the form $C = \underline{\Omega} \times [0, T] \subset \mathbb{R}^n \times \mathbb{R}^+_0$, with $\underline{\Omega}$ a bounded domain. The derivative itself can be done by in the classical way using [51], Chap. IX, Parag. 7. For the problem at hands, the boundedness of the operator, it is enough to study the convolution terms

$$\int_C \partial_{x_j} E^\epsilon_+(x-z, t-s)u(z,s)dzds$$

and

$$\int_C \partial_t E^\epsilon_+(x-z, t-s)u(z,s)dzds.$$

For the kernels of these convolutions we have

$$
\begin{aligned}
&\partial_t(E_+^\epsilon(x-z,t-s)) \\
&= \underbrace{\partial_t e_+^\epsilon(x-z,t-s)}_{(F)} \left[\frac{x-z}{2(\epsilon+i)(t-s)} + \mathfrak{f}\left(\frac{n}{2(t-s)} - \frac{|x-z|^2}{4(\epsilon+i)(t-s)^2}\right) + \mathbf{k}\mathfrak{f}^\dagger\right] \\
&\quad + e_+^\epsilon(x-z,t-s) \underbrace{\partial_t \left[\frac{x-z}{2(\epsilon+i)(t-s)} + \mathfrak{f}\left(\frac{n}{2(t-s)} - \frac{|x-z|^2}{4(\epsilon+i)(t-s)^2}\right) + \mathbf{k}\mathfrak{f}^\dagger\right]}_{(G)},
\end{aligned} \tag{3.28}
$$

$$
\begin{aligned}
&\partial_{x_k}(E_+^\epsilon(x-z,t-s)) \\
&= \underbrace{\partial_{x_k} e_+^\epsilon(x-z,t-s)}_{(D)} \left[\frac{x-z}{2(\epsilon+i)(t-s)} + \mathfrak{f}\left(\frac{n}{2(t-s)} - \frac{|x-z|^2}{4(\epsilon+i)(t-s)^2}\right) + \mathbf{k}\mathfrak{f}^\dagger\right] \\
&\quad + e_+^\epsilon(x-z,t-s) \underbrace{\partial_{x_k} \left[\frac{x-z}{2(\epsilon+i)(t-s)} + \mathfrak{f}\left(\frac{n}{2(t-s)} - \frac{|x-z|^2}{4(\epsilon+i)(t-s)^2}\right) + \mathbf{k}\mathfrak{f}^\dagger\right]}_{(E)},
\end{aligned} \tag{3.29}
$$

where

$$
\begin{aligned}
(D) &= -\frac{(\epsilon+i)e_k x_k}{2(\epsilon^2+1)(t-s)} e_+^\epsilon(x-z,t-s), \\
(E) &= \frac{-1}{2(\epsilon+i)(t-s)} + \mathfrak{f}\frac{-(x_k-z_k)}{2(\epsilon+i)(t-s)^2}, \\
(F) &= \left[-\frac{n}{2(t-s)^{\frac{n}{2}+1}} + \frac{(\epsilon+i)|x-z|^2}{4(\epsilon^2+1)(t-s)^2}\right] e_+^\epsilon(x-z,t-s),
\end{aligned}
$$

and

$$
(G) = -\frac{x-z}{2(\epsilon+i)(t-s)^2} + \mathfrak{f}\left(-\frac{n}{(t-s)^2} + \frac{|x-z|^2}{2(\epsilon+i)(t-s)^3}\right).
$$

Each of these kernels can be written as $\frac{1}{t-s}\varphi(x-z,t-s)$, with a function φ which behaves like the fundamental solution. In a similar way as in the proof of Theorem3.2.5 we can prove φ in $L_p(C)$. This fact combined with the Theorem of Calderon and Zygmund (see [51], Chap. XI, Parag. 3.) allow us to conclude that

$$
||\partial_t(T_-^\epsilon u)||_{L_p(C)} \leq K_1 ||u||_{L_p(C)}, \tag{3.30}
$$

where K_1 is a constant . In a similar manner

$$
||\partial_{x_j}(T_-^\epsilon u)||_{L_p(C)} \leq K_2\, ||u||_{L_p(C)}. \tag{3.31}
$$

Now it remains to extend the previous inequalities to an arbitrary bounded domain $\Omega \subset \mathbb{R}^n \times \mathbb{R}_0^+$. To do that, we consider a space-time cylinder C such that $\Omega \subset C$. We extend our function $u \in L_p(\Omega)$ to

$$\tilde{u}(x,t) = \begin{cases} u(x,t), & (x,t) \in \Omega \\ 0 & (x,t) \in C \setminus \Omega \end{cases}$$

Here we have

$$\partial_t \int_C E_+^\epsilon(x-z,t-s)\tilde{u}(z,s)dzds = \partial_t \int_\Omega E_+^\epsilon(x-z,t-s)u(z,s)dzds.$$

Since the first term defines a bounded operator from $L_p(C)$ to $L_p(C)$, the second represents also a bounded operator from $L_p(\Omega)$ to $L_p(C)$ and, due to

$$\int_\Omega |v(z,s)|^p dzds \leq \int_C |v(z,s)|^p dzds,$$

to $L_p(\Omega)$.

■

Taking into account the previous results, we can prove the continuity of the regularized Teodorescu operator for bounded domains.

Theorem 3.2.12 *For $1 < p < +\infty$, the regularized Teodorescu operator*

$$T_-^\epsilon : L_p(\Omega) \to W_p^1(\Omega),$$

is continuous.

This is now a direct consequence of Theorems 3.2.11 and 3.2.10.

The following result is a important property of the regularized Teodorescu operator.

Theorem 3.2.13 *The regularized Teodorescu operator T_-^ϵ is the right inverse of the regularized parabolic-type Dirac operator D_-^ϵ, i.e., for a function $u \in L_p(\Omega)$ we have the following equality:*

$$D_-^\epsilon T_-^\epsilon u = u.$$

Proof: Under these conditions we have in the distributional sense

$$\begin{aligned} D_-^\epsilon T_-^\epsilon u &= -D_-^\epsilon \left(E_+^\epsilon * u\right) \\ &= -[D_-^\epsilon E_+^\epsilon] * u \\ &= -[(D_* - \mathbf{k}\mathfrak{f}^\dagger)E_+^\epsilon] * u \end{aligned} \tag{3.32}$$

We recall that $D_* = D + \mathfrak{f}\partial_t$, the homogeneous part of our Dirac operator. Hence

$$\begin{aligned} D_-^\epsilon T_-^\epsilon u &= -[(e_+^\epsilon D_+^\epsilon)(-D_* - \mathbf{k}\mathfrak{f}^\dagger)] * u \\ &= -[-e_+^\epsilon (D_+^\epsilon)^2] * u \\ &= \delta * u \\ &= u. \end{aligned}$$

■

Based on expression (3.24) we have the following definition

Definition 3.2.14 *Let $u \in W_p^{1-\frac{1}{p}}(\partial\Omega)$. We define the regularized Cauchy-Bitsadze operator as*

$$F_-^\epsilon u(x,t) = \int_{\partial\Omega} E_+^\epsilon(x-z, t-r) d\sigma_{z,r} u(z,r), \quad (x,t) \notin \partial\Omega. \tag{3.33}$$

Using (3.26) and (3.33) we can rewrite (3.24) as

$$F_-^\epsilon u = u - T_-^\epsilon D_-^\epsilon u,$$

whenever $u \in W_p^{1-\frac{1}{p}}(\Omega)$, and for every $1 < p < +\infty$.

In the following results we prove some properties of the operator (3.33).

Theorem 3.2.15 *For every $\epsilon > 0$, the regularized Cauchy-Bitsadze operator (3.33) verifies*

$$(D_-^\epsilon F_-^\epsilon) u = 0,$$

for every $u \in W_p^{1-\frac{1}{p}}(\partial\Omega)$.

Proof: Let us consider a function $u \in W_p^{1-\frac{1}{p}}(\partial\Omega)$, with $(x,t) \in \Omega$. We have

$$\begin{aligned}
(D_-^\epsilon F_-^\epsilon u)(x,t) &= \int_{\partial\Omega} D_-^\epsilon E_+^\epsilon(x-z,t-s)d\sigma_{z,s}u(z,s) \\
&= \int_{\partial\Omega} D_-^\epsilon e_+^\epsilon(x-z,t-s)D_+^\epsilon d\sigma_{z,s}u(z,s) \\
&= -\int_{\partial\Omega} e_+^\epsilon(x-z,t-s)D_+^\epsilon D_+^\epsilon d\sigma_{z,s}u(z,s) \\
&= -\int_{\partial\Omega} e_+^\epsilon(x-z,t-s)(-\Delta_x+\mathbf{k}\partial_t)d\sigma_{z,s}u(z,s) \\
&= -\int_{\partial\Omega} \delta_x(x-z)\delta_t(t-s)d\sigma_{z,s}u(z,s) \\
&= 0.
\end{aligned}$$

The last simplification is valid because $(x,t) \in \Omega$ and $(z,r) \in \partial\Omega$, which implies that the difference $(x-z,t-r)$ is always non-zero.

■

Theorem 3.2.16 *The regularized Cauchy-Bitsadze operator is continuous in* $W_p^{a-\frac{1}{p}}(\partial\Omega)$,*with* $a \in \mathbb{N}$, *i.e., the operator*

$$F_-^\epsilon : W_p^{a-\frac{1}{p}}(\partial\Omega) \to W_p^a(\Omega) \cap \ker(D_+^\epsilon(\Omega)),$$

where $1 \leq p < +\infty$ *and* $a \in \mathbb{N}$, *is continuous.*

Proof: For a function $u \in W_p^{a-\frac{1}{p}}(\partial\Omega)$ there exists a function $v \in W_p^a(\Omega)$ such that $\mathrm{tr} v = u$ and by the Borel-Pompeiu formula obtained previously we can say that

$$F_-^\epsilon u = (I - T_-^\epsilon D_-^\epsilon)v.$$

Taking into account the result about the continuity of the regularized Teodorescu operator and the fact that for a function $v \in W_p^a(\Omega)$ we have $(D_-^\epsilon v) \in W_p^a(\Omega)$, we obtain

$$(I - T_-^\epsilon D_-^\epsilon)v \in W_p^a(\Omega).$$

By the Theorem 3.2.15 we have $(D_-^\epsilon F_-^\epsilon)u = (D_-^\epsilon(I - T_-^\epsilon D_-^\epsilon))v = 0$, which implies that $F_-^\epsilon u \in W_p^a(\Omega) \cap \ker(D_-^\epsilon(\Omega))$, for a function $u \in W_p^{a-\frac{1}{p}}(\partial\Omega)$.

■

Finally we use the regularized Cauchy-Bitsadze operator in order to define the following two projectors.

Definition 3.2.17 *For a function $u \in W_p^{1-\frac{1}{p}}(\partial\Omega)$, we define the Plemelj-Sokhotzkij's projectors $\mathbf{P}^\epsilon$ and $\mathbf{Q}^\epsilon$ as*

$$(\mathbf{P}^\epsilon u)(x,t) = n.t. - \lim_{(z,r)\to(x,t)} (F_+^\epsilon u)(z,r) \tag{3.34}$$

and

$$(\mathbf{Q}^\epsilon u)(x,t) = n.t. - \lim_{(y,s)\to(x,t)} (F_+^\epsilon u)(y,s), \tag{3.35}$$

where $(x,t) \in \partial\Omega$, $(z,r) \in \Omega$, $(y,s) \in \text{ext}(\overline{\Omega})$ and the limit is a non-tangential limit.

Since $((\mathbf{P}^\epsilon)^2 u)(x,t) = (\mathbf{P}^\epsilon u)(x,t)$ and $((\mathbf{Q}^\epsilon)^2 u)(x,t) = (\mathbf{Q}^\epsilon u)(x,t)$, for all $(x,t) \in \partial\Omega$, we conclude that (3.34) and (3.35) are indeed projectors.

3.2.3 Hypoelliptic analysis

In this section we use the family of regularized time-dependent operators in order to obtain a generalization of some classical theorems of complex analysis.

Theorem 3.2.18 *For a function $u \in L_p(\Omega)$ is valid the following equality*

$$\int_\Omega (D_-^\epsilon u)(x,t)dxdt = \int_{\partial\Omega} u(x,t)\alpha(x,t)dS_{x,t} - \mathbf{k}\mathfrak{f}^\dagger \int_\Omega u(x,t)dxdt,$$

where $\alpha(x,t)$ is the outward pointing normal unit vector at (x,t).

Proof: Let us consider $u, v \in W_p^1(\Omega)$, with $1 \leq p < +\infty$. By the regularized generic Stokes' formula (3.23) we have

$$\int_{\partial\Omega} v d\sigma_{x,t} u = \int_\Omega [(vD_+^\epsilon)u + v(D_-^\epsilon u)]dxdt.$$

In the previous expression, if we replace v by the constant function 1 and we take into account that $1D_-^\epsilon = -\mathbf{k}\mathfrak{f}^\dagger$, we obtain

$$\begin{aligned}\int_{\partial\Omega} d\sigma_{x,t} u(x,t) &= \int_\Omega [(1D_+^\epsilon)u(x,t) + 1(D_-^\epsilon u)(x,t)]dxdt \\ &= +\mathbf{k}\mathfrak{f}^\dagger \int_\Omega u(x,t)dxdt + \int_\Omega (D_-^\epsilon u)(x,t)dxdt.\end{aligned}$$

If we denote by $\alpha(x,t)$ the outward pointing normal unit vector at (x,t), we finally have

$$\int_{\Omega}(D_{-}^{\epsilon}u)(x,t)dxdt = \int_{\partial\Omega} u(x,t)\alpha(x,t)dS_{x,t} - \mathbf{k}\mathfrak{f}^{\dagger}\int_{\Omega} u(x,t)dxdt.$$

■

Corollary 3.2.19 ***[Cauchy's integral theorem]*** *For a function $u \in L_p(\Omega)\cap \ker(D_{-}^{\epsilon})$, with $1 \leq p < +\infty$, we have the following inequality*

$$\int_{\partial\Omega} u(x,t)\alpha(x,t)dS_{x,t} = \mathbf{k}\mathfrak{f}^{\dagger}\int_{\Omega} u(x,t)dxdt,$$

where $\alpha(x,t)$ is the outward pointing normal unit vector at (x,t).

Also, from the expression (3.24) we obtain

Theorem 3.2.20 ***[Cauchy's integral formula]*** *Consider that Ω has smooth boundary. If $u \in L_p(\Omega)\cap \ker(D_{-}^{\epsilon})$, with $1 \leq p < +\infty$, then we have*

$$(F_{-}^{\epsilon}u)(x,t) = \begin{cases} u(x,t) & in \quad \Omega \\ 0 & in \quad (\mathbb{R}^n\times\mathbb{R}^+)\setminus\overline{\Omega} \end{cases}. \tag{3.36}$$

Corollary 3.2.21 *If $u \in L_p(\Omega)\cap \ker(D_{-}^{\epsilon})$, then u has partial derivatives $\partial_{x_1},\ldots,\partial_{x_n}$ and ∂_t of any order.*

When we are study the stationary case (c.f. [39]) our simple domains are balls centered at $x\in\mathbb{R}^n$ and radius R, i.e. $B_R(x)$. Since we are studying the non-stationary case we need to consider the cylinders as our simple domains. From this point until the end of this subsection, we will define a cylinder center at the point $(x,t)\in\mathbb{R}^n\times\mathbb{R}^+$ with radius R and height T by

$$C_{R,T}(x,t) = \left]t-\frac{T}{2}, t+\frac{T}{2}\right[\times B_R(x),$$

where

$$B_R(x) = \{x\in\mathbb{R}^n : |x-z| < R\} \subset \mathbb{R}^n.$$

Theorem 3.2.22 ***[Mean-value formula]*** *For a function $u \in L_p(\Omega) \cap \ker(D_-^\epsilon)$, with $1 \leq p < \infty$, we can present the following regularized mean-value formula*

$$u(x,t) = \int_{\partial C_{R,T}(x,t)} E_+^\epsilon(x-z,t-r)\alpha(z,r)u(z,r)dS_{z,r},$$

where $\alpha(z,r)$ is the outward pointing normal unit vector the point (x,t).

Proof: From the Cauchy's integral formula (3.36) we have

$$u(x,t) = \int_{\partial C_{R,T}(x,t)} E_+^\epsilon(x-z,t-r)d\sigma_{z,r}u(z,r).$$

By the definition of the cylinder $C_{R,T}(x,t)$, the right hand side of the previous expression is equal to

$$\begin{aligned}&\int_{\partial B_R(x,0)} E_+^\epsilon(x-z,-r)\alpha_1(z,r)dS_{z,r}\\ &\quad+\int_0^T\int_{\partial B_R(x,t)} E_+^\epsilon(x-z,t-r)\alpha_2(z,r)u(z,r)dS_{z,r}dr\\ &\quad+\int_{\partial B_R(x,T)} E_+^\epsilon(x-z,T-r)\alpha_3(z,r)dS_{z,r}.\end{aligned}$$

Since the balls $B_R(x,0)$ and $B_R(x,T)$ are contained in hyperplanes which are parallel to $\mathbb{R}^n$, we immediately conclude that the outward pointing normal unit vectors $\alpha_1(z,r)$ and $\alpha_3(z,r)$, with $(z,r) \in B_R(x,0)$ and $(z,r) \in B_R(x,T)$, have the following coordinates

$$\alpha_1 = (\underbrace{0,...,0}_{n\times},-1) \quad \alpha_3 = (\underbrace{0,...,0}_{n\times},1).$$

In order to obtain the outward pointing normal unit vector α_2 we need to remark that $C^*_{R,T}(x,t)$, for each value of $t \in]0,T[$, is a ball $B_R(x,t)$. In this conditions we conclude that the outward pointing normal unit vector α_2 at the point $(z,t) \in B_R(x,t)$, is given by

$$\alpha_2(z,r) = \left(\frac{z-x}{R}, \frac{t-t}{R}\right) = \left(\frac{z-x}{R}, 0\right).$$

■

With the mean-value formula obtained previously, we can present the following generalizations of some classical results of Complex analysis.

Theorem 3.2.23 ***[Maximum modulus theorem]*** *Suppose that the domain Ω is connected and $u \in L_p(\Omega) \cap \ker(D_-^\epsilon)$, with $1 \leq p < +\infty$ and $\overline{\Omega} = \Omega \cup \partial\Omega$. If there exists some $(z,r) \in \Omega$ with*

$$|u(x,t)| \leq |u(z,r)|, \quad \forall\ (x,t) \in \Omega,$$

then u is a constant function. Conversely if u is a constant function, then there exists some $(z,r) \in \Omega$ such that

$$|u(x,t)| \leq |u(z,r)|, \quad \forall\ (x,t) \in \Omega.$$

Proof: For $(z,r) \in \Omega$ there exists a cylinder $C_{R,T}(z,r) \subset \Omega$. Applying the mean value formula we obtain

$$u(z,r) = \int_{\partial C_{R,T}(z,r)} E_+^\epsilon(z-x, r-t)\alpha(x,t)u(x,t)dS_{x,t},$$

where $\alpha(x,t)$ is the outward pointing normal unit vector at (x,t).

Assume now that $|u(x,t)| < \frac{|u(z,r)|}{\lambda}$, where

$$\lambda = \int_{\partial C_{R,T}(z,r)} |E_+^\epsilon(z-x, r-t)|dS_{x,t},$$

and also assume that u is a not constant function in $C_{R,T}(z,r)$. Then there exists a decomposition of $C_{R,T}(z,r)$ in two sets

$$\begin{aligned} C'_{R,T}(z,r) &= \left\{(x,t) \in C_{R,T}(z,r) : |u(x,t)| = \frac{|u(z,r)|}{\lambda}\right\} \\ C''_{R,T}(z,r) &= \left\{(x,t) \in C_{R,T}(z,r) : |u(x,t)| < \frac{|u(z,r)|}{\lambda}\right\}. \end{aligned}$$

In this conditions, the initial expression yields

$$\begin{aligned} |u(z,r)| &< \int_{\partial C'_{R,T}(z,r)} |E_+^\epsilon(z-x, r-t)|\frac{|u(z,r)|}{\lambda}dS_{x,t} \\ &\quad + \int_{\partial C''_{R,T}(z,r)} |E_+^\epsilon(z-x, r-t)|\frac{|u(z,r)|}{\lambda}dS_{x,t} \\ &= \frac{|u(z,r)|}{\lambda}\int_{\partial C'_{R,T}(z,r) \cup \partial C''_{R,T}(z,r)} |E_+^\epsilon(z-x, r-t)|dS_{x,t} \\ &= |u(z,r)|. \end{aligned}$$

This is a contradiction. Hence on $\partial C_{R,T}(z,r)$ we have $|u(x,t)| = |u(z,r)|$. If we choose a smaller cylinder $C_{R',T'}(z,r)$ ($R' < R,\ T' < T$) we obtain the same absurd. Therefore, $|u(x,t)| = |u(z,r)|$ in the whole cylinder $C_{R,T}(z,r)$. Since Ω is connected we get immediately $|u(x,t)| = const.$ on Ω and for the continuity of $|u(x,t)|$ such that also on $\overline{\Omega}$. It remains to show that $u(x,t)$ is also constant. From $|u|^2 = const.$ we conclude

$$D_-^\epsilon |u|^2 = D_- |u|^2 = -\mathbf{k}\mathfrak{f}^\dagger |u|^2,$$

and also

$$\begin{aligned}
(-\Delta - \mathbf{k}\partial_t)|u|^2 &= (D_-^\epsilon D_-^\epsilon)|u|^2 \\
&= -D_-^\epsilon \mathbf{k}\mathfrak{f}^\dagger |u|^2 \\
&= -D_*(\mathbf{k}\mathfrak{f}^\dagger |u|^2) + \mathbf{k}^2 (\mathfrak{f}^\dagger)^2 |u|^2 \\
&= 0 + 0 \\
&= 0.
\end{aligned}$$

Since the components of a Clifford left regular function are harmonic one we get that $D_-^\epsilon u = 0$, and consequently u is a constant function.

■

Corollary 3.2.24 *If the domain Ω is connected and $u \in L_p(\Omega) \cap \ker(D_-^\epsilon)$, with $1 \leq p < +\infty$ then*

$$\sup_{(x,t)\in\overline{\Omega}} |u(x,t)| = \sup_{(x,t)\in\partial\Omega} |u(x,t)|.$$

3.2.4 $\mathbf{L_p}-$decomposition

As we saw previously, an useful method in the study of partial differential equations (PDEs) is the factorization of second-order operators in terms of first-order ones. Under some conditions, this factorization procedure allow us to obtain an orthogonal decomposition of the L_2-space where one of the components is the kernel of the corresponding first-order operator. This decomposition, when possible, is one of the most interesting aspects of complex and hypercomplex analysis with quite useful applications, specially in the theory of PDE's. In [39] such orthogonal decomposition was used to study boundary-value problems of mathematical physics over bounded domains in scales of Hilbert spaces. The treatment of non-stationary cases, however, carries extra difficulties due to the time-evolution and the nature of the singularities of the corresponding fundamental solution. The aim of this subsection is to obtain a L_p-decomposition for the backward case of the Schrödinger equation. We present an immediate application to the resolution of the linear Schrödinger problem.

Taking into account the ideas presented in [19], we can present the following results about the decomposition of L_p-spaces.

Theorem 3.2.25 *The space $L_p(\Omega)$, $1 \leq p < +\infty$ allows the following decomposition*

$$L_p(\Omega) = L_p(\Omega) \cap ker\left(D_-^\epsilon\right) \oplus D_-^\epsilon\left(\overset{\circ}{W}{}_p^1(\Omega)\right), \tag{3.37}$$

for all $\epsilon > 0$, and we can define the following projectors

$$\begin{aligned} P_-^\epsilon : \quad L_p(\Omega) &\to L_p(\Omega) \cap ker\left(D_-^\epsilon\right) \\ Q_-^\epsilon : \quad L_p(\Omega) &\to D_-^\epsilon\left(\overset{\circ}{W}{}_p^1(\Omega)\right), \end{aligned}$$

where P_-^ϵ and Q_-^ϵ are called Bergman projectors.

Proof: Since the operator D_-^ϵ is hypoelliptic, we can say that the operator $-\Delta - \mathbf{k}\partial_t$, with $\mathbf{k} = \frac{\epsilon+i}{\epsilon^2+1}$, is also hypoelliptic. In this conditions and taking into account [66], we can guarantee the existence and uniqueness of the operator solution $(-\Delta - \mathbf{k}\partial_t)_0^{-1}$ for problem

$$\left\{ \begin{array}{rcl} (-\Delta - \mathbf{k}\partial_t)u &=& f \text{ in } \Omega \\ u &=& 0 \text{ in } \partial\Omega \end{array} \right. .$$

As a first step we take a look at the intersection of the two subspaces $D_-^\epsilon\left(\overset{\circ}{W}{}_p^1(\Omega)\right)$ and $L_p(\Omega) \cap \ker\left(D_-^\epsilon\right)$.

Consider a function u in $\left[L_p(\Omega) \cap \ker\left(D_-^\epsilon\right)\right] \cap D_-^\epsilon\left(\overset{\circ}{W}{}_p^1(\Omega)\right)$. It is immediate that $D_-^\epsilon u = 0$, in Ω, and also that there exists a function $v \in \overset{\circ}{W}{}_p^1(\Omega)$ such that $D_-^\epsilon v = u$ and $(-\Delta - \mathbf{k}\partial_t)v = 0$, and this due to $u \in D_-^\epsilon\left(\overset{\circ}{W}{}_p^1(\Omega)\right)$.

Applying $(-\Delta - \mathbf{k}\partial_t)_0^{-1}$, we get $v = 0$ and, consequently, $u = 0$, i. e., the intersection of this subspaces contains only the zero function. Therefore, our sum is a direct sum.

Now, let us consider $u \in L_p(\Omega)$. We have

$$u_2 = D_-^\epsilon(-\Delta - \mathbf{k}\partial_t)_0^{-1} D_-^\epsilon u \ \in \ D_-^\epsilon \left(\overset{\circ}{W_p^1} (\Omega) \right).$$

Applying D_-^ϵ to $u_1^\epsilon = u - u_2^\epsilon$, we obtain

$$\begin{aligned} D_-^\epsilon u_1 &= D_-^\epsilon u - D_-^\epsilon u_2 \\ &= D_-^\epsilon u - D_-^\epsilon D_-^\epsilon(-\Delta - \mathbf{k}\partial_t)_0^{-1} D_-^\epsilon u \\ &= D_-^\epsilon u - (-\Delta - \mathbf{k}\partial_t)(-\Delta - \mathbf{k}\partial_t)_0^{-1} D_-^\epsilon u \\ &= D_-^\epsilon u - D_-^\epsilon u \\ &= 0, \end{aligned}$$

i.e., $D_-^\epsilon u_1 \in \ker\left(D_-^\epsilon\right)$.

■

Corollary 3.2.26 *For the case of $p = 2$ the decomposition is orthogonal.*

Proof: The right linear sets $\mathcal{A} = L_2(\Omega) \cap \ker(D_-)$ and $\mathcal{B} = L_2(\Omega) \ominus \mathcal{A}$ are subspaces of $L_2(\Omega)$. For every function $u \in L_2(\Omega)$ we have that $T_-^\epsilon u \in W_2^1(\Omega)$. From this it follows that there exists a function $v \in W_2^1(\Omega)$ with $u = D_-^\epsilon v$. Let $u = D_-^\epsilon v \in \mathcal{B}$. Then, we have for all $g \in \mathcal{A}$

$$\int_\Omega \overline{D_- v} g \, dxdt = 0,$$

which proves the orthogonality of our decomposition.

■

Our next aim is to extend the previous L_p-decomposition to one depending on the original parabolic-type Dirac operator D_-. In order to obtain this, we initially show a refinement of the previous convergence result presented for the family of regularized fundamental solutions $(E_+^\epsilon)_{\epsilon>0}$.

Theorem 3.2.27 *For all $1 \leq p \leq 2$ we have the following weak convergence, in $W_p^{-\frac{n}{2}-1}(\Omega)$,*

$$\left\langle E_+^\epsilon, \varphi \right\rangle \ \to \ \left\langle E_+, \varphi \right\rangle, \quad \varphi \in W_p^{\frac{n}{2}+1}(\Omega),$$

when $\epsilon \to 0$.

Proof: Given $\varphi \in W_p^{\frac{n}{2}+1}(\Omega)$, we have

$$\begin{aligned}
\left|\langle E_+^\epsilon, \varphi\rangle - \langle E_+, \varphi\rangle\right| &= 2^{\frac{np}{2}} \left| \int_\Omega \left[\left(E_+^\epsilon(x,t) - E_+(x,t) \right) \overline{\varphi(x,t)} \right]_0 dxdt \right| \\
&= 2^{\frac{np}{2}} \left| \int_\Omega \left[\left(D_+^\epsilon e_+^\epsilon(x,t) - D_+ e_+(x,t) \right) \overline{\varphi(x,t)} \right]_0 dxdt \right| \\
&\leq \underbrace{2^{\frac{np}{2}} \int_\Omega \left| (D_+^\epsilon - D_+) e_-^\epsilon(x,t) \right| |\varphi(x,t)| \, dxdt}_{(H)} \\
&\quad + \underbrace{2^{\frac{np}{2}} \int_\Omega \left| e_+^\epsilon(x,t) - e_+(x,t) \right| |D_+\varphi(x,t)| \, dxdt}_{(J)} \qquad (3.38)
\end{aligned}$$

Hence

$$\begin{aligned}
(H) &\leq 2^{\frac{np}{2}} 2^{-\frac{np}{2}} ||(D_+^\epsilon - D_+) e_-^\epsilon||_{L_p(\Omega)} \, ||\varphi||_{L_p(\Omega)} \\
&= ||(D_+^\epsilon - D_+) e_+^\epsilon||_{L_p(\Omega)} \, ||\varphi||_{L_p(\Omega)},
\end{aligned}$$

and, by Theorem 3.2.3, we conclude that this term tends to 0 as $\epsilon \to 0$. Also

$$\begin{aligned}
(J) &= 2^{-\frac{np}{2}} \int_\Omega \left| e_+^\epsilon(x,t) - e_+(x,t) \right| |D_+\varphi(x,t)| \, dxdt \\
&\leq 2^{-\frac{np}{2}} \int_\Omega \left| \frac{\epsilon + i}{(\epsilon + i)^{\frac{n}{2}}} - \frac{i}{i^{\frac{n}{2}}} \right| \frac{H(t)}{(4\pi t)^{\frac{n}{2}}} |D_+\varphi(x,t)| \, dxdt,
\end{aligned}$$

which converges to zero when $\epsilon \to 0$ if $\varphi \in W_p^{\frac{n}{2}+1}(\Omega)$.

■

With this results we are in conditions to present the following convergence results.

Theorem 3.2.28 *The family of regularized Teodorescu operators T_-^ϵ converges weakly to the following Teodorescu operator*

$$T_- u(x_0, t_0) = -\int_\Omega E_+(x - x_0, t - t_0) u(x,t) dxdt, \qquad (3.39)$$

with $(x_0, t_0) \notin \partial\Omega$, in $W_p^{-\frac{n}{2}-1}(\Omega)$, for all $u \in L_p(\Omega)$, and for all $1 \leq p \leq 2$.

Proof: Let $u \in L_p(\Omega)$. Taking into account the previous Theorem we have, for every $\varphi \in$

$W_p^{\frac{n}{2}+1}(\Omega)$, that

$$\begin{aligned}
\lim_{\epsilon\to 0^+}\left|\langle T_-^\epsilon u,\, \varphi\rangle\right| &= \lim_{\epsilon\to 0^+}\left|\langle E_+^\epsilon * u,\, \varphi\rangle\right| \\
&= \left|\langle \lim_{\epsilon\to 0^+} E_+^\epsilon,\, u*\varphi\rangle\right| \\
&= \left|\langle E_+,\, u*\varphi\rangle\right| \\
&= \left|\langle E_+ * u,\, \varphi\rangle\right| \\
&= \left|\langle T_-, \varphi\rangle\right|.
\end{aligned}$$

■

Theorem 3.2.29 *The family of projectors Q_-^ϵ is a fundamental family in $W_p^{-\frac{n}{2}-1}(\Omega)$, for all $1 \le p \le 2$.*

Proof: Let us start with the proof of the convergence. Consider $u \in L_p(\Omega)$ and $\varphi \in W_p^{\frac{n}{2}+1}(\Omega)$, where $1 \le p < +\infty$. Since for all $\epsilon > 0$, $(Q_-^\epsilon)^2 = Q_-^\epsilon$ and $Q_-^\epsilon(P_-^\epsilon u) = 0$, we have for any $\epsilon_1, \epsilon_2 > 0$

$$\begin{aligned}
\left|\langle Q_-^{\epsilon_1}u - Q_-^{\epsilon_2}u,\, \varphi\rangle\right| &= \left|\langle Q_-^{\epsilon_1}(P_-^{\epsilon_1}u + Q_-^{\epsilon_1}u) - Q_-^{\epsilon_2}(P_-^{\epsilon_1}u + Q_-^{\epsilon_1}u),\, \varphi\rangle\right| \\
&= \left|\langle Q_-^{\epsilon_1}u - Q_-^{\epsilon_2}P_-^{\epsilon_2}u - Q_-^{\epsilon_2}Q_-^{\epsilon_1}u,\, \varphi\rangle\right| \\
&\le \underbrace{\left|\langle Q_-^{\epsilon_2}P_-^{\epsilon_1}u,\, \varphi\rangle\right|}_{(K)} + \underbrace{\left|\langle (I - Q_-^{\epsilon_2})Q_-^{\epsilon_1}u,\, \varphi\rangle\right|}_{(L)}.
\end{aligned}$$

For $P_-^\epsilon : L_p(\Omega) \to \ker(D_-)$ the projectors defined previously, we have for the term (K)

$$\begin{aligned}
\left|\langle Q_-^{\epsilon_2}P_-^{\epsilon_1}u,\, \varphi\rangle\right| &= \left|\langle Q_-^{\epsilon_2}(F_-^{\epsilon_1}P_-^{\epsilon_1} - Q_-^{\epsilon_2}F_-^{\epsilon_2})P_-^{\epsilon_1}\rangle\right| \\
&= \left|\langle Q_-^{\epsilon_2}(I - T_-^{\epsilon_1}D_-^{\epsilon_1} - (I - T_-^{\epsilon_2}D_-^{\epsilon_2}))P_-^{\epsilon_1}u,\, \varphi\rangle\right| \\
&= \left|\langle Q_-^{\epsilon_2}(T_{-1}^{\epsilon}D_-^{\epsilon_1} - T_-^{\epsilon_2}D_-^{\epsilon_2})P_-^{\epsilon_1}u,\, \varphi\rangle\right| \\
&= \left|\langle Q_-^{\epsilon_2}(T_-^{\epsilon_1}(D_-^{\epsilon_1} - D_-^{\epsilon_2}) + (T_-^{\epsilon_1} - T_-^{\epsilon_2})D_-^{\epsilon_2})P_-^{\epsilon_1}u,\, \varphi\rangle\right|
\end{aligned}$$

Taking into account Theorems 3.2.3 and 3.2.28, we get the weak convergence of (K), in $W_p^{-\frac{n}{2}-1}(\Omega)$ for all $1 \le p < +\infty$, of the right hand side of the last expression to zero. Finally, since $Q_-^{\epsilon_1}u \in D_-\left(\overset{\circ}{W}{}_p^1(\Omega)\right)$, there exists $g \in \overset{\circ}{W}{}_p^1(\Omega)$ such that $u = D_-^\epsilon g$. Therefore, (L)

becomes

$$\begin{aligned}
\left|\langle (I-Q_-^{\epsilon_2})Q_-^{\epsilon_1}u,\,\varphi\rangle\right| &= \left|\langle (I-Q_-^{\epsilon_2})D_-^{\epsilon}g,\,\varphi\rangle\right| \\
&= \left|\langle D_-^{\epsilon_1}g - Q_-^{\epsilon_2}D_-^{\epsilon_1}g + D_-^{\epsilon_2}g - D_-^{\epsilon_2}g\,\varphi\rangle\right| \\
&= \left|\langle Q_-^{\epsilon_2}(D_-^{\epsilon}g - D_-g) + (D_-g - D_-^{\epsilon}g),\,\varphi\rangle\right| \\
&= \left|\langle (D_-g - D_-^{\epsilon}g)(I-Q_-^{\epsilon_1}),\,\varphi\rangle\right|.
\end{aligned}$$

By Theorem 3.2.3 we conclude that the last expression goes to zero as $\epsilon \to 0$.

■

Now it remains to prove that Q_- is idempotent. Hereby, we have

$$Q_-^2 = \lim_{\epsilon\to 0}(Q_-^{\epsilon})^2 = \lim_{\epsilon\to 0} Q_-^{\epsilon} = Q_-.$$

Theorem 3.2.30 *For a given $f \in L_p(\Omega)$, with $1 \leq p \leq 2$, consider the solutions (u) for the problem*

$$\begin{cases} (-\Delta - \mathbf{k}\partial_t)u &= f \\ u|_\Gamma &= 0 \end{cases}, \tag{3.40}$$

for each $\epsilon > 0$.

Then, the family of such solutions (u) is a fundamental family in $W_p^{-\frac{n}{2}-1}(\Omega)$, for all $1 \leq p < +\infty$. Moreover, $(D_-^{\epsilon}u)$ is a fundamental family in $W_p^{-\frac{n}{2}-1}(\Omega)$.

Proof: Let us consider $\varphi \in W_p^{\frac{n}{2}+1}(\Omega)$, $f \in L_p(\Omega)$ and a family of functions (u), such that $u \in D_-^{\epsilon}(\Omega)$ with $\epsilon > 0$, and $\epsilon_1, \epsilon_2 > 0$. Since the elements of the family are solution of the problem (3.40), we have that $u = T_-^{\epsilon}Q_-^{\epsilon}T_-^{\epsilon}f$ (for more details about this assertion see [17]). Then

$$\begin{aligned}
|\langle u^{\epsilon_1} - u^{\epsilon_2},\,\varphi\rangle| &= \left|\langle T_-^{\epsilon_1}Q_-^{\epsilon_1}T_-^{\epsilon_1}f - T_-^{\epsilon_2}Q_-^{\epsilon_2}T_-^{\epsilon_2}f,\,\varphi\rangle\right| \\
&= \left|\langle \left(T_-^{\epsilon_1}Q_-^{\epsilon_1}T_-^{\epsilon_1} - T_-^{\epsilon_2}Q_-^{\epsilon_2}T_-^{\epsilon_2}\right)f,\,\varphi\rangle\right| \\
&\leq \left|\langle \left(T_-^{\epsilon_1}Q_-^{\epsilon_1}\left(T_-^{\epsilon_1} - T_-^{\epsilon_2}\right)\right)f,\,\varphi\rangle\right| \\
&\quad + \left|\langle \left(\left(T_-^{\epsilon_1} - T_-^{\epsilon_2}\right)Q_-^{\epsilon_2}T_-^{\epsilon_2}\right)f,\,\varphi\rangle\right| \\
&\quad + \left|\langle \left(T_-^{\epsilon_1}\left(Q_-^{\epsilon_1} - Q_-^{\epsilon_2}\right)T_-^{\epsilon_2}\right)f,\,\varphi\rangle\right|.
\end{aligned}$$

By the Theorems 3.2.28 and 3.2.29 we conclude that the right hand side of the last inequality tends to zero when $\epsilon_1, \epsilon_2 \to 0$.

Taking into account Theorem 3.2.25 we can guarantee that there exists a function $f \in L_p(\Omega)$ such that

$$D_-^{\epsilon_1} u^{\epsilon_1} = Q_-^{\epsilon_1} T_-^{\epsilon_1} f \quad \text{and} \quad D_-^{\epsilon_2} u^{\epsilon_2} = Q_-^{\epsilon_2} T_-^{\epsilon_2} f,$$

which implies that

$$\begin{aligned} \left|\left\langle \left(Q_-^{\epsilon_1} T_-^{\epsilon_1} - Q_-^{\epsilon_2} T_-^{\epsilon_2}\right) f, \varphi \right\rangle\right| \quad &\leq \quad \left|\left\langle \left(Q_-^{\epsilon_1} \left(T_-^{\epsilon_1} - T_-^{\epsilon_2}\right)\right) f, \varphi \right\rangle\right| \\ &\quad + \left|\left\langle \left(\left(Q_-^{\epsilon_1} - Q_-^{\epsilon_2}\right) T_-^{\epsilon_2}\right) f, \varphi \right\rangle\right|. \end{aligned}$$

By the Theorems 3.2.28 and 3.2.29 we conclude that the right hand side of the previous expression converges weakly to zero when $|\epsilon_1 - \epsilon_2| \to 0$, in $W_p^{-\frac{n}{2}-1}(\Omega)$, for all $1 \leq p < +\infty$.

■

This result can be refined. In fact, denote by $u_2 \in W_p^{-\frac{n}{2}-1}(\Omega)$ the function limit of the Cauchy family studied. Taking into account Theorem 3.2.30, we can guarantee the existence of $f \in L_p(\Omega)$, with $1 \leq p \leq 2$, such that

$$(-\Delta - i\partial_t) u_2 = f \quad \text{and} \quad (-\Delta - i\partial_t) u_2^\epsilon = f,$$

with $u_2|_\Gamma = 0 = u_2^\epsilon|_\Gamma$.

Since $(-\Delta - i\partial_t)^{-1}$ exists and it is unique in (for more details see [66]), we can establish the following equality

$$u_2 - u_2^\epsilon = (-\Delta - i\partial_t)^{-1} \left((-\Delta - \mathbf{k}\partial_t) - (-\Delta - i\partial_t)\right) u_2^\epsilon,$$

which implies that

$$||u_2 - u_2^\epsilon||_{L_p(\Omega)} \leq ||(-\Delta - i\partial_t)^{-1}||_{L_1(\Omega)} \; ||(-\Delta - \mathbf{k}\partial_t) - (-\Delta - i\partial_t)||_{L_1(\Omega)} \; ||u_2^\epsilon||_{L_q(\Omega)}.$$

Since $||(-\Delta - \mathbf{k}\partial_t) - (-\Delta - i\partial_t)||_{L_1(\Omega)}$ converges to zero when $\epsilon \to 0$, we conclude that the right hand side of the last expression also converges to zero. This fact implies that $u_2 \in L_p(\Omega)$.

Moreover, we can guarantee, for $1 \leq p \leq 2$, that

(i) For any two elements $u_2^{\epsilon_1}$ and $u_2^{\epsilon_2}$ of the fundamental family studied in Theorems 3.2.29 and 3.2.30, there exists functions $g_2^{\epsilon_1}, g_2^{\epsilon_2} \in \overset{\circ}{W}{}_p^1(\Omega)$ such that

$$u_2^{\epsilon_1} = D_-^{\epsilon_1} g_2^{\epsilon_1} \quad \text{and} \quad u_2^{\epsilon_2} = D_-^{\epsilon_2} g_2^{\epsilon_1}$$

and

$$\begin{aligned} ||D_-^{\epsilon_2}(g_2^{\epsilon_1} - g_2^{\epsilon_2})||_{L_p(\Omega)} &= ||D_-^{\epsilon_2} g_2^{\epsilon_1} - D_-^{\epsilon_1} g_2^{\epsilon_1} + D_-^{\epsilon_1} g_2^{\epsilon_2} - D_-^{\epsilon_2} g_2^{\epsilon_2}||_{L_p(\Omega)} \\ &\leq ||\left(D_-^{\epsilon_2} - D_-^{\epsilon_1}\right) g_2^{\epsilon_1}||_{L_p(\Omega)} \\ &\qquad + ||u_2^{\epsilon_1} - u_2^{\epsilon_2}||_{L_p(\Omega)}. \end{aligned}$$

By Theorems 3.2.3 and 3.2.30 and the above considerations, we conclude that the right hand side of the previous expression converges to zero, when $|\epsilon_1 - \epsilon_2| \to 0$, i.e.

$$||D_-^{\epsilon_2}(g_2^{\epsilon_1} - g_2^{\epsilon_2})||_{L_p(\Omega)} \to 0, \quad \text{when } |\epsilon_1 - \epsilon_2| \to 0.$$

Since $||D_-^{\epsilon}||_{L_1(\Omega)} \to ||D_-||_{L_1(\Omega)} < \infty$, when $\epsilon \to 0$, we conclude that $g \to g_2^{\epsilon_2} + C$, when $|\epsilon_1 - \epsilon_2| \to 0$ and $\epsilon_1, \epsilon_2 \to 0$, where $C \in \ker(D_-)$.

In this conditions we showed that for any function $u \in L_p(\Omega)$, there exists an function $v \in \overset{\circ}{W}{}_p^1(\Omega)$ such that $u = D_- v$.

(ii) Suppose that there exist two functions $g_1, g_2 \in \overset{\circ}{W}{}_p^1(\Omega)$, such that

$$u = D_- g_1 \quad \text{and} \quad u = D_- g_2,$$

for the same function $u \in L_p(\Omega)$. We have

$$\begin{aligned} (-\Delta - i\partial_t) g_1 = (-\Delta - i\partial_t) g_2 \quad &\Leftrightarrow \quad g_1 = (-\Delta - i\partial_t)^{-1} (-\Delta - i\partial_t) g_2 \\ &\Leftrightarrow \quad g_1 = g_2, \end{aligned}$$

which proves our assertion.

Theorem 3.2.31 *For each $u \in L_p(\Omega)$, the family of $P_-^{\epsilon} u$ converges to $\hat{u}$ in $\ker(D_{x,-it}^{\epsilon}) \cap L_p(\Omega)$, for all $\epsilon > 0$ and $1 \leq p \leq 2$.*

Proof: The proof is made in three steps: consider $\varphi \in W_p^{\frac{n}{2}+1}(\Omega)$, a function $u \in L_p(\Omega)$, and a family of function (u_1^ϵ), where $u_1^\epsilon \in \ker(D_-^\epsilon) \cap L_p(\Omega)$ with $\epsilon > 0$, with $1 \leq p \leq 2$.

Let $\epsilon_1,\, \epsilon_2 > 0$. Taking into account the decomposition presented in Theorem 3.2.25 we have for $u_1^{\epsilon_1},\, u_1^{\epsilon_2} \in \ker(D_-^{\epsilon_1}),\, \ker(D_-^{\epsilon_2})$

$$\begin{aligned} |\langle u_1^{\epsilon_1} - u_1^{\epsilon_2},\, \varphi\rangle| &= |\langle (u - u_2^{\epsilon_1}) - (u - u_2^{\epsilon_2}),\, \varphi\rangle| \\ &\leq |\langle u_2^{\epsilon_2} - u_2^{\epsilon_1},\, \varphi\rangle|\,, \end{aligned}$$

where $u_2^{\epsilon_1}$ and $u_2^{\epsilon_1}$ are elements of the fundamental family (u_2^ϵ), where $u_2^\epsilon \in D_-^\epsilon(\overset{\circ}{W}{}_p^1(\Omega))$ for $\epsilon > 0$. Taking into account Theorem 3.2.30 we conclude that the right hand side of the last expression converges weakly to zero, in $W_p^{-\frac{n}{2}-1}(\Omega)$, when $|\epsilon_1 - \epsilon_2| \to 0$.

This proves (P_-^ϵ) to be a fundamental family in $W_p^{-\frac{n}{2}-1}(\Omega)$.

Moreover, using the techniques and arguments presented for the family $D_-^\epsilon u$, with $\epsilon > 0$, after Theorem 3.2.30, we can refine our conclusion and therefore, prove that the function limit is in $L_p(\Omega)$.

Finally, let us denote by u_1 the function limit of this fundamental family. For a given $\varphi \in W_p^{\frac{n}{2}+1}(\Omega)$, with $1 \leq p \leq 2$, we have

$$\begin{aligned} |\langle D_- u_1,\, \varphi\rangle| &= \left|\langle D_- u_1 - D_-^\epsilon u_1^\epsilon,\, \varphi\rangle\right| \\ &\leq |\langle D_-(u_1 - u_1^\epsilon),\, \varphi\rangle| + \left|\langle (D_- - D_-^\epsilon) u_1^\epsilon(x,t),\, \varphi\rangle\right|. \end{aligned}$$

Theorems 3.2.31 and 3.2.3 guarantee that, respectively, the first and second term of the right hand side of the last expression converges to 0 when $\epsilon \to 0$.

■

In resume, for each $u \in L_p(\Omega)$, we have $u = P_-^\epsilon u + Q_-^\epsilon u$. Also, we proved that

$$\begin{aligned} Q_-^\epsilon u &\to Q_- u \\ Q_-^2 u &= Q_- u, \end{aligned}$$

which implies that Q_- is a projector and that we can define a projector P_- as

$$P_- u = u - Q_- u,$$

with $P_- u \in \ker(D_-) \cap L_p(\Omega)$.

In this conditions we can generalize the decomposition presented in the beginning of this section by the following result

Theorem 3.2.32 *For $1 \leq p \leq 2$, it is valid the following decomposition*

$$L_p(\Omega) = (L_p(\Omega) \cap \ker(D_-)) \oplus D_-(\overset{\circ}{W}{}_p^1(\Omega)).$$

Moreover, we can define the following projectors

$$\begin{aligned} P_- : \quad L_p(\Omega) \quad & \rightarrow L_p(\Omega) \cap ker\,(D_-) \\ Q_- : \quad L_p(\Omega) \quad & \rightarrow D_- \left(\overset{\circ}{W}{}_p^1(\Omega) \right), \end{aligned}$$

where P_- and Q_- are usually call Bergman projectors.

Proof: Let us denote by $(-\Delta - i\partial_t)_0^{-1}$ the solution operator of the problem

$$\left\{ \begin{array}{rcl} (-\Delta - i\partial_t)u & = & f \quad in \ \Omega \\ u & = & 0 \quad on \ \partial\Omega \end{array} \right. .$$

As first step we take a look at the intersection of the two subspaces $D_- \left(\overset{\circ}{W}{}_p^1 (\Omega) \right)$ and $L_p(\Omega) \cap \ker\,(D_-)$.

Consider $u \in L_p(\Omega) \cap \ker\,(D_-) \cap D_- \left(\overset{\circ}{W}{}_p^1 (\Omega) \right)$. It is immediate that $D_- u = 0$ and also, because $u \in D_- \left(\overset{\circ}{W}{}_p^1 (\Omega) \right)$, there exists a function $v \in \overset{\circ}{W}{}_p^1 (\Omega)$ with $D_- v = u$ and $(-\Delta - i\partial_t)v = 0$.

Since $(-\Delta - i\partial_t)_0^{-1} f$ is unique (see [66]) we get $v = 0$ and, consequently, $u = 0$, i.e., the intersection of this subspaces contains only the zero function. Therefore, our sum is a direct sum.

Now let $u \in L_p(\Omega)$. Then we have

$$u_2 = D_-(-\Delta - i\partial_t)_0^{-1} D_- u \ \in \ D_- \left(\overset{\circ}{W}{}_p^1 (\Omega) \right).$$

Let us now apply D_- to the function $u_1 = u - u_2$. This result in

$$\begin{aligned} D_- u_1 &= D_- u - D_- u_2 \\ &= D_- u - D_- D_- (-\Delta - i\partial_t)_0^{-1} D_- u \\ &= D_- u - (-\Delta - i\partial_t)(-\Delta - i\partial_t)_0^{-1} D_- u \\ &= D_- u - D_- u \\ &= 0, \end{aligned}$$

i.e., $D_- u_1 \in \ker(D_-)$. Because $u \in L_p(\Omega)$ was arbitrary chosen our decomposition is a decomposition of the space $L_p(\Omega)$.

■

We end this subsection, with an immediate application of the operator T_- and the projector D_- in the resolution of the linear Schrödinger problem with boundary data.

Theorem 3.2.33 *Let $f \in L_p(\Omega),\ 1 < p \leq 2$. The solution of the problem*

$$\begin{cases} (-\Delta - i\partial_t) u &= f \quad in \quad \Omega \\ u &= 0 \quad on \quad \partial\Omega \end{cases}$$

is given by $u = T_- Q_- T_- f$.

Proof: The proof of this theorem is based on the properties of the operator T_- and of the projector Q_+. Because T_- is the right inverse of D_+, we get

$$D_-^2 u = D_-(Q_- T_- f) = D_-(T_- f) = f.$$

■

Chapter 4

The non-linear Schrödinger problem

"Quantum mechanics is very impressive, but hardly brings us any closer to the secrets of the Old One.

I am any rate convinced that He does play dice."

Albert Einstein

If we want to apply the Schrödinger equation for a specified problem, for example in the description of non-relativistic quantum systems, we need to solve a differential equation with a boundary condition and determinate the eigenvalues and eigenfunctions of that problem. Unfortunately, only in few situations we can solve the Schrödinger equation exactly, and therefore numerical methods are needed.

Recently, the finite difference method has been applied for solving the linear Schrödinger equation (see [63]). In this method, the Schrödinger equation is discretized using central finite difference in time and in space. In order to obtain solutions, we need to perform two simulations using an initial impulse function. In first simulation, we determine the impulse response of the problem, which under the action of the Fourier transform, is used to obtain the eigenvalues of eigenfrequencies. In second simulation, we use the eigenfrequencies combined with the discrete Fourier transform to obtain the eigenfunctions.

In [39], the authors proposed different strategies to solve boundary value problems based on the study of existence, uniqueness, representation and regularity of the solutions, with the help of an operators calculus. In there, the authors introduced also the necessary basic ideas for a discrete counterpart of the continuous treatment of boundary value problems via a discrete operator calculus which leads to a well-adapted numerical approach. An explicit discrete version of the Borel-Pompeiu formula was presented for $n = 3$. The ideas introduced in [39] were further developed in [37] and [38], where finite difference potential methods were developed in lattice domains based on the concept of discrete fundamental solutions for the difference Dirac operator. This generalizes the work of Ryabenkji in [57]. A numerical application of this theory for the case of incompressible stationary Navier-Stokes equations was presented in [31].

The aim of this chapter is to combine Witt basis with finite difference approximations in order to develop a discrete calculus operator that allow us to obtain and implement a numerical scheme for the NLS problem. In this sense, the chapter is structured as follows: in the first section we will proved the existence and uniqueness of solution of the NLS problem and we present a iterative method to solve it. In Section 4.2, we use a quaternionic matrix representation of the Witt basis combined with finite difference and time dependent operators to describe the discrete fundamental solution of the discrete Schrödinger operator. In Section 4.3, we study the convergence of the discrete fundamental solution to the continuous correspondent, both in the implicit and the explicit cases. These conclusions allow the study of the convergence of the discrete operators to the correspondent continuous one. In Subsection 4.3.3 we introduce a convergent discrete iterative method to solve our NLS problem and we present some simple numerical examples to show the consistency and stability of our algorithm.

All the results presented in this chapter can be founded in [13], [15], [18] and [30].

4.1 Resolution of the NLS problem via an iterative method

The name “non-linear Schrödinger equation” (NLS) originates from a formal analogy with the Schrödinger equation of quantum mechanics. In this context a non-linear potential arises in the “mean field” description of the interacting particles, hence its name. The NLS equation can be related with “filamentation instability” phenomena that can be interpreted in the context of non-linear optics, where in the usual situations, the wave modulation is essentially time-independent. When the NLS equation is considered in the wave context, the second-order linear operator, which describes the dispersion and diffraction of the wave-packet, is not necessary elliptic, and the non-linearity arises from the sensitivity of the refractive index to the medium of the wave amplitude. The phenomenon of the wave-packet contraction can also occur in a one-dimensional setting. The non-linear development of the modulational instability depends, however, strongly on the space dimension. When the modulation is purely one-dimensional, it leads to the formation of solitonic structures resulting from an exact balance between the dispersive and non-linear effects. In higher dimensions, in contrast, the non-linearity dominates when the initial conditions are large enough in a suitable norm, resulting a blow-up of the wave amplitude, if additional physical effects like dissipation do not intervene to arrest the process. Since a spatial contraction of the wave packet takes place together with the amplitude blowup, the phenomenon if often called wave collapse in the physical literature. This is a basic mechanism to produce transfer of energy from a large to small scales, thus permitting dissipative process to act and to heat the medium, with possible degradation of the material in the case of a dielectric. In plasmas, the collapsing structures, often called "collapsons", will act as a sinks for the wave energy. This phenomenon competes with the more gradual energy transfer to small scales resulting from resonant wave interactions (wave turbulence).

The aims of this section are two: the first one is to prove, via Banach fixed point theorem, the existence and uniqueness of solution for the NLS problem, the second one is to present a convergent iterative method to solve our problem.

4.1.1 Existence and uniqueness of solution

In this section we construct an alternative iterative method for the non-linear Schrödinger equation with non-linearity and we study is convergence. This method will we combine some conclusions obtained in Chapter 3 for the Teodorescu and the Bergman projectors with the resolution of the linear problem presented in the end of the same chapter.

Let us remark that the considered non-linear equation is not the usual, in the sense that we are considering $\mathbb{C}_n-$valued functions instead of complex-valued function.

Consider the (generalized) non-linear Schrödinger problem:

$$\begin{cases} -\Delta u - i\partial_t u + |u|^2 u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{4.1}$$

where $|u|^2 = \sum_A |u_A|^2$. We can rewrite (4.1) as

$$D_-^2 u + M(u) = 0, \tag{4.2}$$

where $M(u) = |u|^2 u - f$. It is easy to see that

$$u = -T_- Q_- T_-(M(u)) \tag{4.3}$$

is a solution of (4.2) by means of direct application of D_-^2 to both sides of the equation.

We remark that for a function u such that for each t fixed $u(\cdot,t) \in W_2^1(\underline{\Omega})$ and for each x fixed $u(x,\cdot) \in W_2^2([0,T))$, we get

$$||D_- u|| = ||Q_- T_- M(u)|| = ||T_- M(u)||.$$

We now prove that (4.3) can be solved by the convergent iterative method

$$u_m = -T_- Q_- T_-(M(u_{m-1})). \tag{4.4}$$

In order to guarantee that we are in the conditions of the Banach point fix theorem, we need to establish some norm estimations. Initially we have that

$$\begin{aligned} ||u_m - u_{m-1}|| &= ||T_- Q_- T_- [M(u_{m-1}) - M(u_{m-2})]|| \\ &\leq C_1 ||M(u_{m-1}) - M(u_{m-2})||, \end{aligned} \tag{4.5}$$

where $C_1 = ||T_- Q_- T_-|| = ||T_-||^2$.

We now estimate the factor $||M(u_{m-1}) - M(u_{m-2})||$. We get

$$\begin{aligned} &||M(u_{m-1}) - M(u_{m-2})|| = |||u_{m-1}|^2 u_{m-1} - |u_{m-2}|^2 u_{m-2}|| \\ &\leq |||u_{m-1}|^2 (u_{m-1} - u_{m-2})|| + |||u_{m-1} - u_{m-2}|^2 u_{m-2}|| \\ &\leq 2^{n+1} ||u_{m-1} - u_{m-2}|| \left(||u_{m-1}||^2 + ||u_{m-2}|| ||u_{m-1} - u_{m-2}|| \right). \end{aligned}$$

We assume $\mathcal{K}_m := 2^{n+1} \left(||u_{m-1}||^2 + ||u_{m-2}|| ||u_{m-1} - u_{m-2}|| \right)$. We get

$$||u_m - u_{m-1}|| \leq C_1 \mathcal{K}_m ||u_{m-1} - u_{m-2}||.$$

Moreover, we have additionally that

$$\begin{aligned} ||u_m|| &= ||T\_Q\_T\_M(u_{m-1})|| \\ &\leq 2^{n+1}C_1||u_{m-1}||^3 + C_1||f|| \end{aligned} \tag{4.6}$$

holds.

In order to prove that indeed we have a contraction we need to study the auxiliary inequality

$$2^{n+1}C_1||u_{m-1}||^3 + C_1||f|| \leq ||u_{m-1}||,$$

that is,

$$||u_{m-1}||^3 - \frac{||u_{m-1}||}{2^{n+1}C_1} + \frac{||f||}{2^{n+1}} \leq 0. \tag{4.7}$$

The analysis of (4.7) will be made considering two cases:

Case I: When $||u_{m-1}|| \geq 1$, we can establish the following inequality in relation to (4.7)

$$||u_{m-1}||^2 - \frac{||u_{m-1}||}{3 \cdot 2^{n+1}} + \frac{||f||}{2^{n+1}} \leq ||u_{m-1}||^3 - \frac{||u_{m-1}||}{2^{n+1}C_1} + \frac{||f||}{2^{n+1}}.$$

Then, from (4.7), we have

$$\begin{aligned} & ||u_{m-1}||^2 - \frac{||u_{m-1}||}{3 \cdot 2^{n+1}} + \frac{||f||}{2^{n+1}} \leq 0 \\ & \Leftrightarrow ||u_{m-1}||^2 - 2\frac{||u_{m-1}||}{6 \cdot 2^{n+1}} + \frac{1}{36 \cdot 2^{2n+2}} + \frac{||f||}{2^{n+1}} - \frac{1}{36 \cdot 2^{2n+2}} \leq 0 \\ & \Leftrightarrow \left(||u_{m-1}|| - \frac{1}{6 \cdot 2^{n+1}} \right)^2 \leq \frac{1}{36 \cdot 2^{2(n+1)}} - \frac{||f||}{2^{n+1}} = \frac{1}{2^{n+1}} \left(\frac{1}{36 \cdot 2^{n+1}} - ||f|| \right). \end{aligned} \tag{4.8}$$

If $||f|| \leq \frac{1}{36 \cdot 2^{n+1}}$ then

$$\left| ||u_{m-1}|| - \frac{1}{6 \cdot 2^{n+1}} \right| \leq W,$$

where $W = \sqrt{\dfrac{1}{36 \cdot 2^{2(n+1)}} - \dfrac{||f||}{2^{n+1}}}$.

In consequence, if

$$\frac{1}{6 \cdot 2^{m+1}} - W \leq ||u_{m-1}|| \leq \frac{1}{6 \cdot 2^{n+1}} + W$$

then we have from (4.6) the desired inequality

$$||u_m|| \leq ||u_{m-1}||.$$

Furthermore, we have now to study the remaining case. Assuming now that $||u_{m-1}|| \leq \dfrac{1}{6 \cdot 2^{n+1}} - W$, we have

$$||u_m|| \leq 2^{n+1} C_1 \left(\frac{1}{6 \cdot 2^{n+1}} - W \right)^3 + C_1 ||f|| \leq \frac{1}{6 \cdot 2^{n+1}} - W$$

and $||u_{m-1}|| \leq \dfrac{1}{6 \cdot 2^{n+1}} - W$, $||u_{m-2}|| \leq \dfrac{1}{6 \cdot 2^{n+1}} - W$ so that it holds

$$||u_{m-1} - u_{m-2}|| \leq 2 \left(\frac{1}{6 \cdot 2^{n+1}} - W \right).$$

With the previous relations we can estimate the value of $\mathcal{K}_m$

$$\begin{aligned} \mathcal{K}_m &= 2^{n+1} \left(||u_{m-1}||^2 + ||u_{m-2}|| ||u_{m-1} - u_{m-2}|| \right) \\ &\leq 2^{n+1} \left[\left(\frac{1}{6 \cdot 2^{n+1}} - W \right)^2 + 2 \left(\frac{1}{6 \cdot 2^{n+1}} - W \right)^2 \right] \\ &\leq 3 \cdot 2^{n+1} \left(\frac{1}{6 \cdot 2^{n+1}} - W \right) \\ &= \frac{1}{2} - 3 \cdot 2^{n+1} W < \frac{1}{2}, \end{aligned} \tag{4.9}$$

which implies that

$$||u_{m-2}|| \leq R := \frac{1}{3 \cdot 2^{n+1}}.$$

Finally, we have that

$$||u_m - u_{m-1}|| \leq \mathcal{K}_m ||u_{m-1} - u_{m-2}||,$$

with $\mathcal{K}_m < \dfrac{1}{2}$.

Case II: When $||u_{m-1}|| < 1$, we can establish the following inequality

$$||u_{m-1}||^4 - \frac{||u_{m-1}||^2}{3 \cdot 2^{n+1}} + \frac{||f||}{2^{n+1}} \leq ||u_{m-1}||^3 - \frac{||u_{m-1}||}{2^{n+1} C_1} + \frac{||f||}{2^{n+1}}.$$

Then, from (4.7) we have

$$\begin{aligned} & ||u_{m-1}||^4 - \frac{||u_{m-1}||^2}{3 \cdot 2^{n+1}} + \frac{||f||}{2^{n+1}} \leq 0 \\ \Leftrightarrow & \left(||u_{m-1}||^2 - \frac{1}{6 \cdot 2^{n+1}} \right)^2 \leq \frac{1}{36 \cdot 2^{2n+2}} - \frac{||f||}{2^{n+1}}. \end{aligned} \tag{4.10}$$

Again, if $||f|| \leq \dfrac{1}{36 \cdot 2^{n+1}}$ then

$$\left| ||u_{m-1}||^2 - \frac{1}{6 \cdot 2^{n+1}} \right| \leq W,$$

where $W = \sqrt{\dfrac{1}{36 \cdot 2^{2n+2}} - \dfrac{||f||}{2^{n+1}}}$.

As a consequence,

$$\begin{aligned} \frac{1}{6 \cdot 2^{n+1}} - W \leq ||u_{m-1}||^2 \leq \frac{1}{6 \cdot 2^{n+1}} + W \\ \Leftrightarrow \sqrt{\frac{1}{6 \cdot 2^{n+1}} - W} \leq ||u_{m-1}|| \leq \sqrt{\frac{1}{6 \cdot 2^{n+1}} + W} \end{aligned}$$

leads to $||u_m|| \leq ||u_{m-1}||$.

Again, considering now the case of $||u_{m-1}|| \leq \sqrt{\dfrac{1}{6 \cdot 2^{n+1}} - W}$, we obtain

$$||u_m|| \leq 2^{n+1} C_1 \left(\sqrt{\frac{1}{6 \cdot 2^{n+1}} - W} \right)^3 + C_1 ||f|| \leq \sqrt{\frac{1}{6 \cdot 2^{n+1}} - W}$$

and

$$||u_{m-1}|| \leq \sqrt{\frac{1}{6 \cdot 2^{n+1}} - W} \qquad ||u_{m-2}|| \leq \sqrt{\frac{1}{6 \cdot 2^{n+1}} - W} - W$$
$$||u_{m-1} - u_{m-2}|| \leq 2\sqrt{\frac{1}{6 \cdot 2^{n+1}} - W}.$$

With the previous relations we can estimate the value of $\mathcal{K}_m$

$$\begin{aligned} \mathcal{K}_m &= 2^{n+1} \left(||u_{m-1}||^2 + ||u_{m-2}|| ||u_{m-1} - u_{m-2}|| \right) \\ &\leq 2^{n+1} \left[\left(\frac{1}{6 \cdot 2^{n+1}} - W \right) + 2 \left(\frac{1}{6 \cdot 2^{n+1}} - W \right) \right] \\ &= 3 \cdot 2^{n+1} \left(\frac{1}{6 \cdot 2^{n+1}} - W \right) \\ &= \frac{1}{2} - 3 \cdot 2^{n+1} W < \frac{1}{2}, \end{aligned} \tag{4.11}$$

which implies that

$$||u_{m-2}|| \leq R := \frac{1}{3 \cdot 2^{n+1}}.$$

Finally, we have that

$$||u_m - u_{m-1}|| \leq \mathcal{K}_m ||u_{m-1} - u_{m-2}||,$$

with $\mathcal{K}_m < \dfrac{1}{2}$.

The application of the Banach's fixed point to the previous conclusions, results the following theorem

Theorem 4.1.1 *The problem (4.1) has a unique solution u, which for each t fixed $u(\cdot,t) \in W_2^1(\underline{\Omega})$ and for each x fixed $u(x,\cdot) \in W_2^2([0,T))$, if $f \in L_2(\Omega)$ satisfies the condition*

$$||f|| \leq \frac{1}{36 \cdot 2^{n+1}}.$$

Moreover, our iterative method (4.4) converges for each starting point u_0, such that for each t fixed $u_0(\cdot,t) \in W_2^1(\underline{\Omega})$, for each x fixed $u_0(x,\cdot) \in W_2^2([0,T))$ and

$$||u_0|| \leq \frac{1}{6 \cdot 2^{n+1}} + W,$$

with $W = \sqrt{\frac{1}{36 \cdot 2^{2(n+1)}} - \frac{||f||}{2^{n+1}}}$.

4.1.2 Convergent iterative method

The aim of this subsection is to propose an iterative method to solve the cubic Schrödinger equation and to show in what conditions this method convergent. The non-linear Schrödinger problem

$$\begin{cases} -i\partial_t u - \Delta u = M(u) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

where $M(u) = |u|^2 u + f$, with $f \in L_2(\Omega)$, and $|u|^2 = \sum_{j=0}^{3} (u^j)^2$, is equivalent to the problem

$$u = -T_- Q_- T_- M(u) \text{ in } \Omega, \tag{4.12}$$

for which the next theorem proves existence and uniqueness of solution (see [9], [17] for details).

Theorem 4.1.2 *The problem (4.12) has an unique solution given in terms of the iterative method*

$$u_{m+1} = -T_- Q_- T_- M(u_m)$$

if $f \in L_2(\Omega)$ *satisfies the condition*

$$||f||_{L_2} \leq \frac{1}{36 \cdot 2^{n+1}}.$$

Moreover, the iterative method converges for each starting point $u_0 \in \overset{\circ}{W}{}^1_2(\Omega)$ *such that*

$$||u_0||_{L_2} \leq \frac{1}{6 \cdot 2^{m+1}} + W,$$

with $W = \sqrt{\frac{1}{36 \cdot 2^{2(n+1)}} - \frac{||f||_{L_2}}{2^{n+1}}}$.

4.2 Discrete fundamental solution for time-evolution problems

In this section, we want to present an expression for a fundamental solution of the discrete Schrödinger operator. To do this effect we start with a quaternionic matrix representation of the Witt basis (Subsection 4.2.1). This representation, combined with finite differences, allows the construction of the discrete version of the Schrödinger and parabolic-type Dirac operators introduced in the previous chapter (Subsection 4.2.2). Thus, taking into account the ideas presented in [38] and the discrete symbol of the Laplace operator, we present an expression for a discrete fundamental solution of our first and second order operators (Subsection 4.2.4).

4.2.1 Quaternionic matrix representation of the Witt basis

The aim of this subsection is to present the analogous of the Witt basis for the discrete case. For that, we use the matrix representation of the generators of the real quaternions as defined in [39],

$$\mathbf{e}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{e}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\mathbf{e}_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{e}_3 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

as representatives of a discrete version of the spatial basis for the quaternionic case.

Moreover, we consider the elements γ^+ and γ^- which satisfy the following matricial operations.

$$\begin{aligned}
\gamma^{\pm}\begin{pmatrix} A & B \\ C & D \end{pmatrix} &= \begin{pmatrix} A & -B \\ -C & D \end{pmatrix}\gamma^{\pm}, \\
(\gamma^{\pm})^2 &= 0, \\
\gamma^+\gamma^- + \gamma^-\gamma^+ &= id.
\end{aligned} \tag{4.13}$$

Taking into account the properties of the Witt basis presented in Section 3.1.1 we conclude that the elements γ^+ and γ^- are the discrete version of $\mathfrak{f}^\dagger$ and $\mathfrak{f}$, respectively.

4.2.2 Finite differences and time evolution operators

As already stated we want to investigate a finite difference scheme based on the notion of a discrete fundamental solution as described in [37]. We denote by

$$\mathbb{R}^3_h = \{h\underline{m} = (hm_1, hm_2, hm_3), m_l \in \mathbb{Z}\} \quad \text{and} \quad \mathbb{R}^+_\tau = \{k\tau, k \in \mathbb{Z}^+\}$$

equidistant lattices corresponding to space and time discretization, respectively. For a discrete function $u : \mathbb{R}^3_h \times \mathbb{R}^+_\tau \to \mathbb{C}^4 \sim \mathbb{C} \otimes \mathbb{H}$, $u(h\underline{m}, k\tau) = (u^0, u^1, u^2, u^3)$, we have the finite difference approximation for the stationary Dirac operators given by

$$D_h^{-+}u = \begin{pmatrix} -\partial_h^{-1}u^1 - \partial_h^{-2}u^2 - \partial_h^{-3}u^3 \\ \partial_h^{-1}u^0 - \partial_h^{3}u^2 + \partial_h^{2}u^3 \\ \partial_h^{-2}u^0 + \partial_h^{3}u^1 - \partial_h^{1}u^3 \\ \partial_h^{-3}u^0 - \partial_h^{2}u^1 + \partial_h^{1}u^2 \end{pmatrix}, \qquad D_h^{+-}u = \begin{pmatrix} -\partial_h^{1}u^1 - \partial_h^{2}u^2 - \partial_h^{3}u^3 \\ \partial_h^{1}u^0 - \partial_h^{-3}u^2 + \partial_h^{-2}u^3 \\ \partial_h^{2}u^0 + \partial_h^{-3}u^1 - \partial_h^{-1}u^3 \\ \partial_h^{3}u^0 - \partial_h^{-2}u^1 + \partial_h^{-1}u^2 \end{pmatrix},$$

$$uD_h^{-+} = \begin{pmatrix} -\partial_h^{-1}u^1 - \partial_h^{-2}u^2 - \partial_h^{-3}u^3 \\ \partial_h^{-1}u^0 + \partial_h^{3}u^2 - \partial_h^{2}u^3 \\ \partial_h^{-2}u^0 - \partial_h^{3}u^1 + \partial_h^{1}u^3 \\ \partial_h^{-3}u^0 + \partial_h^{2}u^1 - \partial_h^{1}u^2 \end{pmatrix}, \qquad uD_h^{+-} = \begin{pmatrix} -\partial_h^{1}u^1 - \partial_h^{2}u^2 - \partial_h^{3}u^3 \\ \partial_h^{1}u^0 + \partial_h^{-3}u^2 - \partial_h^{-2}u^3 \\ \partial_h^{2}u^0 - \partial_h^{-3}u^1 + \partial_h^{-1}u^3 \\ \partial_h^{3}u^0 + \partial_h^{-2}u^1 - \partial_h^{-1}u^2 \end{pmatrix},$$

where

$$\partial_h^{\pm s}u^j = \frac{(u^j(h\underline{m} \pm he_s, k\tau) - u^j(h\underline{m}, k\tau))}{h}, \; j = 0, 1, 2, 3, \; s = 1, 2, 3,$$

represents the spatial forward/backward difference operators. We remark that these difference Dirac operators factorize the star discretization of the Laplacian, in the sense that

$$D_h^{+-}D_h^{-+} = D_h^{-+}D_h^{+-} = -\Delta_h \mathbf{e}_0 = \left(\sum_{s=1}^{3} \partial_h^{-s}\partial_h^{s}\right)\mathbf{e}_0.$$

Moreover, we also have the following (forward) time difference operator (see [39] and [37])

$$\partial_\tau u^j(h\underline{m}, k\tau) = \frac{u^j(h\underline{m},(k+1)\tau) - u^j(h\underline{m},k\tau)}{\tau}, \; j = 0, \cdots, 3.$$

With the previous definitions we aim to construct a finite difference approximation for the parabolic-type Dirac operator. For this purpose we introduce the matrix representations

$$D_{h,\pm\tau} = \begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix}\gamma^+ \pm \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix}\gamma^-. \tag{4.14}$$

Using the properties of the previous operators and taking into account the multiplication rules (4.13) we obtain the following relation

$$\begin{aligned}
(D_{h,\pm\tau})^2 &= \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix}\gamma^+ \pm \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix}\gamma^-\right]^2 \\
&= \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix}\right]^2 + \left[\begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix}\gamma^+\right]^2 + \left[\begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix}\gamma^-\right]^2 \\
&\quad + \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix}\gamma^+ + \begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 + \end{pmatrix}\gamma^+\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix}\right] \\
&\quad \pm \left[\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix}\begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix}\gamma^- + \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 + \end{pmatrix}\gamma^-\begin{pmatrix} \mathbf{0} & D_h^{-+} \\ D_h^{+-} & \mathbf{0} \end{pmatrix}\right] \\
&\quad \pm \left[\begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix}\gamma^+\begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 \end{pmatrix}\gamma^- + \begin{pmatrix} i\mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\mathbf{e}_0 + \end{pmatrix}\gamma^-\begin{pmatrix} \partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \partial_\tau \mathbf{e}_0 \end{pmatrix}\gamma^+\right] \\
&= \begin{pmatrix} -\Delta_h & \mathbf{0} \\ \mathbf{0} & -\Delta_h \end{pmatrix} + \left[\begin{pmatrix} \mathbf{0} & \partial_\tau D_h^{-+} \\ \partial_\tau D_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & -\partial_\tau D_h^{-+} \\ -\partial_\tau D_h^{+-} & \mathbf{0} \end{pmatrix}\right]\gamma^+ \\
&\quad \pm \left[\begin{pmatrix} \mathbf{0} & iD_h^{-+} \\ iD_h^{+-} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & -iD_h^{-+} \\ -iD_h^{+-} & \mathbf{0} \end{pmatrix}\right]\gamma^- \pm \begin{pmatrix} i\partial_\tau \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & i\partial_\tau \mathbf{e}_0 \end{pmatrix}(\gamma^+\gamma^- + \gamma^-\gamma^+) \\
&= (-\Delta_h \pm i\partial_\tau)\begin{pmatrix} \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{e}_0 \end{pmatrix},
\end{aligned} \tag{4.15}$$

i.e., these operators factorize the difference discretization of our time evolution operator $(-\Delta \pm i\partial_t)$. Moreover, due to the fact that the above finite difference operator D_h^{-+}, D_h^{+-}, and ∂_τ are approximations of the Dirac operator D and the time partial derivative operator ∂_t, respectively (see [41]), we have that (4.14) are a finite difference approximations for the parabolic-type Dirac operators $D_\pm = D + \mathfrak{f}\partial_t \pm i\mathfrak{f}^\dagger$.

4.2.3 Discrete symbol of the Laplace operator

Now, we consider the discrete Fourier transform introduced by Stummel (for details, see [62], [38]) with respect to x,

$$(\mathcal{F}_h u)(\xi,\cdot) \;=\; \begin{cases} \frac{h^3}{(2\pi)^{\frac{3}{2}}} \sum_{h\underline{m}\in\mathbb{Z}^3} u(h\underline{m},\cdot)\exp(ih < \underline{m},\xi >) & \text{for } \xi \in Q_h \\ \\ 0 & \text{otherwise} \end{cases},$$

where $Q_h = \left\{\xi = (\xi_1,\xi_2,\xi_3) \in \mathbb{R}^3 : \; -\frac{\pi}{h} < \xi_1,\xi_2,\xi_3 < +\frac{\pi}{h}\right\}$. We remark that $\mathcal{F}_h$ maps a discrete function $u = u(h\underline{m})$ into a continuous function $\hat{u}(\xi) = \mathcal{F}_h u(\xi)$ with support in the cube Q_h. Furthermore, we have $\mathcal{F}_h\delta_h(\xi) = \chi_h(\xi)$ with χ_h being the characteristic function of Q_h.

In order to obtain an expression for $e_{h,-\tau}$, we need to introduce the abbreviation for the symbol of the discrete Laplace operator (for its computation we refer to [41] or [61])

$$-d^2 = -\frac{4}{h^2}\left(\sin^2\left(\frac{h\xi_1}{2}\right) + \sin^2\left(\frac{h\xi_2}{2}\right) + \sin^2\left(\frac{h\xi_3}{2}\right)\right),$$

that is, d^2 satisfies

$$\mathcal{F}_h(-\Delta_h u)(\xi) = d^2(\mathcal{F}_h u)(\xi).$$

4.2.4 Discrete fundamental solutions

On the basis of the ideas presented in [41], we introduce the discrete fundamental solution for the Schrödinger difference operator $-i\partial_\tau - \Delta_h$ as

$$e_{h,+\tau}(h\underline{m},k\tau) = iH(k\tau)\left(1 + i\tau\Delta_h\right)^{k-1}\delta_h(h\underline{m}), \tag{4.16}$$

where H denotes the Heaviside function and

$$\delta_h(h\underline{m}) = \begin{cases} \frac{1}{h^3} & \text{if} \quad h\underline{m} = \mathbf{0} \\ 0 & \text{if} \quad h\underline{m} \neq \mathbf{0} \end{cases}, \quad \delta_\tau(k\tau) = \begin{cases} \frac{1}{\tau} & \text{if} \quad k\tau = 0 \\ 0 & \text{if} \quad k\tau \neq 0 \end{cases},$$

are the discrete analogues of the Dirac delta function in $\mathbb{R}_h^3$ and $\mathbb{R}_\tau^+$, respectively. Easy calculations show that, indeed, we have

$$(i\partial_\tau - \Delta_h)e_{h,+\tau}(h\underline{m}, k\tau) = e_{h,+\tau}(i\partial_\tau - \Delta_h)(h\underline{m}, k\tau) = \delta_\tau(k\tau)\delta_h(h\underline{m}). \tag{4.17}$$

By the factorization property (4.15), we have for the discrete fundamental solution of the operator $D_{h,+\tau}$ the function

$$E_{h,+\tau} = e_{h,+\tau}D_{h,+\tau}. \tag{4.18}$$

Moreover, straightforward calculations give the following matrix representation for the discrete fundamental solution $E_{h,-\tau}$

$$E_{h,+\tau}(h\underline{m}, k\tau) =$$
$$\left[\begin{pmatrix} \mathbf{0} & D_h^{-+}e_{h,+\tau} \\ D_h^{+-}e_{h,+\tau} & \mathbf{0} \end{pmatrix} + \partial_\tau e_{h,+\tau}\begin{pmatrix} \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{e}_0 \end{pmatrix}\gamma^+ + ie_{h,+\tau}\begin{pmatrix} \mathbf{e}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{e}_0 \end{pmatrix}\gamma^-\right]. \tag{4.19}$$

However, it remains to prove that the discrete fundamental solutions $e_{h,+\tau}$ and $E_{h,+\tau}$ are indeed an approximation of the fundamental solutions (3.18) and (3.19). This will be done in the next section.

4.3 Discrete operator calculus

In this section, we prove the convergence of our discrete fundamental solution to the continuous one. This converge give us the possibility of study the behavior of the discrete integral operators on a given refined grid and, thus, to establish a convergent numerical scheme for the cubic NLS equation. We finish this section with some simple numerical examples.

In order to simplify the notation, no distinction will be made between the function $u : \Omega \to \mathbb{C}^4$ and its restriction $u = u(h\underline{m}, k\tau)$ to the lattice $\Omega_{h,\tau} = \Omega \cap (\mathbb{R}_h^3 \times \mathbb{R}_\tau^+)$, this distinction being clear from the context. We will consider the following l_p-norm $l_p(\Omega)$ is the discrete space of all functions u such that

$$||u||_{l_p(\Omega)} = \left(\sum_{(h\underline{m},\tau k)\in\Omega} h^3\tau|g(h\underline{m}, \tau k)|^p\right)^{\frac{1}{p}} < \infty.$$

4.3.1 Behavior of the discrete fundamental solution

We now study the behavior of the discrete fundamental solution (4.17) when h and τ tend to zero and we prove that it converges in l_1-sense to the restriction to the grid of the fundamental solution (3.18), for the explicit and implicit case.

Explicit Case

In this section, we aim at existence of an expression and convergence results in the l_1-norm for a fundamental solution of the operator present in the explicit equation (4.24). We remark that we use here the forward time difference operator as a replacement for the continuous time-derivative in the Schrödinger operator.

For the part of existence we use a constructive procedure. We begin by constructing the discrete symbol of our discrete Schrödinger operator, which we will use to build an expression for $E_{h,+\tau}$. Applying our discrete Fourier transform to (4.24) we get

$$\begin{aligned} i(d^2\mathcal{F}_h e_{h,+\tau} + i\partial_\tau \mathcal{F}_h e_{h,+\tau})(\xi,\tau k) &= \partial_\tau(\mathcal{F}_h e_{h,+\tau})(\xi,\tau k) + id^2(\mathcal{F}_h e_{h,+\tau})(\xi,\tau k) \\ &= \frac{1}{(2\pi)^{\frac{3}{2}}}\delta_\tau(\tau k)\chi_h(\xi), \end{aligned}$$

where $\chi_h(\xi)$ denotes the characteristic function of the cube Q_h. This equation has the solution

$$\left(\mathcal{F}_h e_{h,+\tau}\right)(\xi,\tau k) = \frac{i}{2\pi} H(\tau k)\left(1 - i\tau d^2\right)^{k-1}\chi_h(\xi). \tag{4.20}$$

The inverse of the discrete Fourier transform is given by $\mathcal{F}_h^{-1} = R_h\mathcal{F}$, the restriction to the lattice $\mathbb{R}_h^3$ of the usual Fourier transform $\mathcal{F}$ (see e.g. [41], [61]).

Hence, from (4.20) we get

$$\begin{aligned} e_{h,+\tau}(h\underline{m},\tau k) &= \mathcal{F}_h^{-1}\left(\frac{i}{2\pi} H(\tau k)\left(1 - i\tau d^2\right)^{k-1}\chi_h(\xi)\right) \\ &= iH(\tau k)\left(\left(1 - i\tau\Delta_h\right)^{k-1}\delta_h\right)(h\underline{m}) \end{aligned} \tag{4.21}$$

as an expression for a fundamental solution of the explicit discrete time-dependent Schrödinger operator.

Now, we aim at an estimate of the norm $||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h\times\mathbb{R}_\tau^+)}$. By the properties of the norm we have

$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}^+_\tau)} \leq$$
$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]0,T_0]_\tau)} + ||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]T_0,+\infty]_\tau)}, \tag{4.22}$$

for an arbitrary $T_0 > 0$. This has the advantage of splitting the above expression into two terms which can be more easily treated individually. First, we consider the case of the bounded in time interval, that is to say, the first term on the right hand side. Afterwards, we give an estimate for the second term. The combination of these two estimates will provide us with an estimate for the original norm. Of course, this will be a rather crude estimate. However, we will prove later that a T_0 can be found which ensures both previous estimates to be non-negative and such that their sum goes to zero with the mesh sizes h and τ.

Case of the interval bounded in time

In this section we will study the behavior of

$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]0,T_0]_\tau)}.$$

The expression (4.21) can be rewritten as

$$e_{h,+\tau}(h\underline{m}, \tau k) = \left(1 + \frac{6\tau i}{h^2}\right) e_{h,+\tau}(h\underline{m}, \tau k) + \frac{\tau i}{h^2}\left[\sum_{s=1}^{3} e_{h,+\tau}(h\underline{m} \pm h e_s, \tau k)\right].$$

From this we get

$$\begin{aligned} ||e_{h,+\tau}(\cdot, \tau k)||_{l_1(\mathbb{R}^3_h)} &= ||(1 - i\tau\Delta_h)^{k-1}\delta_h||_{l_1(\mathbb{R}^3_h)} \\ &= \sum_{\underline{m} \in \mathbb{Z}^3_h} |(1 - i\tau\Delta_h)^{k-1}\delta_h(h\underline{m})| h^3, \end{aligned}$$

for all k larger or equal then 1. We apply the binomial formula and the fact that one has $\sum_{\underline{m} \in \mathbb{Z}^3_h} \Delta_h^s \delta_h(h\underline{m}) = 0$ whenever $s \geq 1$. Then, after a convenient re-arrangement of the sum's index we obtain

$$||e_{h,+\tau}(\cdot, \tau k)||_{l_1(\mathbb{R}^3_h)} = \sum_{\underline{m} \in \mathbb{Z}^3_h} \delta_h(h\underline{m}) h^3 = 1.$$

Without loss of generality we assume $T_0 = \tau k_0$, with $k_0 \in \mathbb{N}$. Summing up over the time-steps we obtain the estimate

$$||e_{h,+\tau}||_{l_1(G_h \times]0,T_0]_\tau)} \leq \sum_{k=1}^{k_0} ||e_{h,+\tau}(\cdot, \tau k)||_{l_1(\mathbb{R}^3_h)} \tau \leq \sum_{k=1}^{k_0} \tau = T_0. \tag{4.23}$$

Now, we introduce the continuous fundamental solution

$$e_+(x,t) = \frac{iH(t)}{(4i\pi t)^{\frac{3}{2}}} \exp\left(-\frac{i|x|^2}{4t}\right) \tag{4.24}$$

of the backward continuous Schrödinger operator.

For l_1-norm of its restriction to the space grid the estimate we have

$$\begin{aligned} ||R_h e_+(\cdot,t)||_{l_1(G_h)} &\leq H(t) \sum_{h\underline{m}\in G_h} \left|\frac{i}{(4i\pi t)^{\frac{3}{2}}}\right| \left|\exp\left(\frac{-ih^2|\underline{m}|^2}{4t}\right)\right| h^3 \\ &= \frac{H(t)}{(4\pi t)^{\frac{3}{2}}} \sum_{h\underline{m}\in G_h} h^3 \\ &= \frac{H(t)}{(4\pi t)^{\frac{3}{2}}} Vol(G_h), \end{aligned}$$

with $Vol(G_h) = \sum_{h\underline{m}\in G_h} h^3$. Hence, we get for its space-time-discretization the following estimate

$$\begin{aligned} ||R_\tau R_h e_+||_{l_1(G_h\times]0,T_0]_\tau)} &= \sum_{k=1}^{k_0} \frac{Vol(G_h)}{(4\pi\tau k)^{\frac{3}{2}}} \tau \\ &= \frac{Vol(G_h)}{(4\pi)^{\frac{3}{2}} \ \tau^{\frac{1}{2}}} \sum_{k=1}^{k_0} \frac{1}{k^{\frac{3}{2}}} \\ &\leq Vol(G_h) \frac{T_0 + k_0^2}{(4\pi)^{\frac{3}{2}}}. \end{aligned} \tag{4.25}$$

From (4.25) and (4.23) we conclude

$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h\times]0,T_0]_\tau)} \leq T_0 + T_0 \frac{Vol(G_h)}{(4\pi)^{\frac{3}{2}}} + T_0 \frac{Vol(G_h)k_0^2}{(4\pi)^{\frac{3}{2}}}. \tag{4.26}$$

For simplicity of sake, we denote $C_1(h) = \frac{Vol(G_h)}{(4\pi)^{\frac{3}{2}}}$, and $C_2(h,k_0) = \frac{Vol(G_h)k_0^2}{(4\pi)^{\frac{3}{2}}}$. Moreover, both tend to zero when $h \to 0$. We remark that the obtained estimate is a bad one, specially for a rather large T_0. However, the estimate of the remaining term in the second hand side of (4.22) will compensate this deficiency.

Case of the interval unbounded in time

In the following we study

$$||e_{h,\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h)}, \qquad k \in \mathbb{N},$$

where $\tau k \in \mathbb{R}_\tau^+$ satisfies $\tau k > T_0$.

In order to guarantee the convergence of the integrals and series that will appear in our future computations, we need to consider the regularized fundamental solutions of the regularized Schrödinger operators

$$e_+^\epsilon(x,t) = \frac{(\epsilon+i)H(t)}{(4\pi(\epsilon+i)t)^{\frac{3}{2}}} \exp\left(\frac{-(\epsilon+i)|x|^2}{4(\epsilon^2+1)t}\right), \quad \epsilon > 0, \tag{4.27}$$

which converge to the continuous fundamental solution (3.17) in distributional sense as $\epsilon \to 0$ (see [14] for more details). In here we will omit a general discussion regarding discrete spaces of distributions because we are interested in convergence results in norms as strong as possible. Hence, we only investigate if our fundamental solution (4.21), $e_{h,+\tau}$, belongs to the space $l_1(\mathbb{R}_h^3 \times \mathbb{R}_\tau^+)$.

We have

$$\begin{aligned}
&||e_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h)} \\
=&\sum_{h\underline{m}\in G_h} |e_{h,+\tau}(h\underline{m},\tau k) - R_\tau R_h e_+(h\underline{m},\tau k)| \; h^3 \\
\leq& Vol(G_h) \max_{h\underline{m}\in G_h} |e_{h,+\tau}(h\underline{m},\tau k) - R_\tau R_h e_+(h\underline{m},\tau k)| \\
=& Vol(G_h) \max_{h\underline{m}\in G_h} \left|(R_h\mathcal{F}\mathcal{F}_h e_{h,+\tau})(h\underline{m},\tau k) - (R_\tau R_h \mathcal{F}\mathcal{F}^{-1}e_+)(h\underline{m},\tau k)\right| \\
\leq& Vol(G_h) \max_{h\underline{m}\in G_h} \Bigg[\underbrace{\left|(R_\tau R_h\mathcal{F}\mathcal{F}^{-1}e_+^\epsilon)(h\underline{m},\tau k) - (R_\tau R_h \mathcal{F}\mathcal{F}^{-1}e_+)(h\underline{m},\tau k)\right|}_{(I)} \\
&+ \underbrace{\left|(R_h\mathcal{F}\mathcal{F}_h e_{h,+\tau})(h\underline{m},\tau k) - (R_\tau R_h \mathcal{F}\mathcal{F}^{-1}e_+^\epsilon)(h\underline{m},\tau k)\right|}_{(II)} \Bigg]
\end{aligned} \tag{4.28}$$

By the convergence of the regularized fundamental solution e_+^ϵ to the continuous one, we get immediately that the term (I) converges to zero as ϵ goes to zero. For the remaining term (II) we have

$$\begin{aligned}
(II) \;&\leq\; \left|\frac{1}{2\pi}\int_{\mathbb{R}^3} \left[(\mathcal{F}_h e_{h,+\tau})(x,\tau k) - (R_\tau \mathcal{F}^{-1}e_+^\epsilon)(x,\tau k)\right] \; \exp\left(-i < x, h\underline{m} >\right) dx\right| \\
&\leq\; \frac{1}{2\pi} \int_{\mathbb{R}^3} \left|(\mathcal{F}_h e_{h,+\tau}(x,\tau k) - (R_\tau \mathcal{F}^{-1}e_+^\epsilon)(x,\tau k)\right| \; \left|\exp\left(-i < x, h\underline{m} >\right)\right| dx \\
&=\; \frac{1}{2\pi} \, ||(\mathcal{F}_h e_{h,+\tau})(\cdot,\tau k) - (R_\tau \mathcal{F}^{-1}e_+^\epsilon)(\cdot,\tau k)||_{L_1(\mathbb{R}^3)}.
\end{aligned}$$

Again, we split the study of this expression in two cases, namely, the norms evaluated at $\mathbb{R}^3\backslash Q_h$ and Q_h. For the integral over $\mathbb{R}^3\backslash Q_h$ we have

$$\begin{aligned} ||(\mathcal{F}_h e_{h,+\tau})(\cdot,\tau k) - (R_\tau \mathcal{F}^{-1} e_+^\epsilon)(\cdot,\tau k)||_{L_1(\mathbb{R}^3\backslash Q_h)} &= ||(R_\tau \mathcal{F}^{-1} e_+^\epsilon)(\cdot,\tau k)||_{L_1(\mathbb{R}^3\backslash Q_h)} \\ &= \frac{H(\tau k)}{2(2\pi)^{\frac{3}{2}}\tau k \epsilon^{\frac{1}{2}}} \left|\left| \exp\left(-\frac{|\xi + \frac{\vec{1}}{\epsilon}|^2 t}{\epsilon}\right)\right|\right|_{L_1(\mathbb{R}^3\backslash Q_h)}, \end{aligned} \tag{4.29}$$

where $\frac{\vec{1}}{\epsilon} = \left(\frac{1}{\epsilon}, \frac{1}{\epsilon}, \frac{1}{\epsilon}\right)$. Hence,

$$(4.29) \leq \frac{H(\tau k)\epsilon^{\frac{5}{2}}}{(2\pi)^{\frac{3}{2}}(\tau k)^{\frac{7}{2}}} \exp\left(-\frac{\tau k \pi^2}{h^2 \epsilon}\right). \tag{4.30}$$

For the integral over Q_h we get

$$\begin{aligned} &||(\mathcal{F}_h e_{h,+\tau})(\cdot,\tau k) - (R_\tau \mathcal{F}^{-1} e_+^\epsilon)(\cdot,\tau k)||_{L_1(Q_h)} \\ =&\left|\left| \frac{iH(\tau k)}{(2\pi)^{\frac{3}{2}}}(1 - i\tau d^2)^{k-1} - \frac{iH(\tau k)}{2^{\frac{5}{2}}(\pi i)^{\frac{3}{2}} k\tau\epsilon^{\frac{1}{2}}} \exp\left(-\frac{|\xi + \frac{\vec{1}}{\epsilon}|^2}{\epsilon}\right)\right|\right|_{L_1(Q_h)} \\ =&\frac{H(\tau k)}{(2\pi)^{\frac{3}{2}}\ 2\ \tau k\epsilon^{\frac{1}{2}}} \left|\left| 2\tau k\epsilon^{\frac{1}{2}}(1 - i\tau d^2)^{k-1} - \exp\left(-\frac{|\xi + \frac{\vec{1}}{\epsilon}|^2\tau k}{\epsilon}\right)\right|\right|_{L_1(Q_h)} \\ \leq&\frac{H(\tau k)}{(2\pi)^{\frac{3}{2}}\ 2\ \tau k\ \epsilon^{\frac{1}{2}}} \left\{ \underbrace{\left|\left| 2\ \tau k\ \epsilon^{\frac{1}{2}}\ (1 - i\tau d^2)^{k-1} - \exp\left(-\frac{|d + \frac{1}{\epsilon}|^2\tau k}{\epsilon}\right)\right|\right|_{L_1(Q_h)}}_{(III)} \right. \\ &\left. + \underbrace{\left|\left| \exp\left(-\frac{|d + \frac{1}{\epsilon}|^2\tau k}{\epsilon}\right) - \exp\left(-\frac{|\xi + \frac{\vec{1}}{\epsilon}|^2\tau k}{\epsilon}\right)\right|\right|_{L_1(Q_h)}}_{(IV)} \right\}. \end{aligned} \tag{4.31}$$

Now, we shall give estimates for the norms (III) and (IV). We start here with the term (IV), since it is more easy to handle.

Using the Taylor's expansion of d^2 we have

$$\begin{aligned} \left|\xi + \frac{\vec{1}}{\epsilon}\right|^2 - \left|d + \frac{1}{\epsilon}\right|^2 &= \left|\xi + \frac{\vec{1}}{\epsilon}\right|^2 - \frac{4}{h^2}\left(\sum_{i=1}^3 \sin^2\left(\frac{h\left(\xi_i + \frac{1}{\epsilon}\right)}{2}\right)\right) \\ &\leq \frac{h^2}{12}\left(\sum_{i=1}^3 \left(\xi_i + \frac{1}{\epsilon}\right)^4\right) \\ &\leq \frac{h^2}{12}\left|\xi + \frac{\vec{1}}{\epsilon}\right|^4, \end{aligned}$$

and taking into account the fact that $\left|d+\frac{1}{\epsilon}\right|^2 \geq \frac{4\left|\xi+\frac{\vec{1}}{\epsilon}\right|^2}{\pi^2}$ we get

$$\begin{aligned}
\left|\exp\left(-\frac{|d+\frac{1}{\epsilon}|^2\tau k}{\epsilon}\right)-\exp\left(-\frac{\left|\xi+\frac{\vec{1}}{\epsilon}\right|^2\tau k}{\epsilon}\right)\right| &\leq \frac{\tau k}{\epsilon}\left(\left|\xi+\frac{\vec{1}}{\epsilon}\right|^2-\left|d+\frac{1}{\epsilon}\right|^2\right)\exp\left(-\frac{|d+\frac{1}{\epsilon}|^2\tau k}{\epsilon}\right)\\
&\leq \frac{\tau k h^2}{12\epsilon}\left|\xi+\frac{\vec{1}}{\epsilon}\right|^4\exp\left(-\frac{4\left|\xi+\frac{\vec{1}}{\epsilon}\right|^2\tau k}{\pi^2\epsilon}\right)\\
&\leq \frac{\tau k h^2}{6\epsilon}|\xi|^4\exp\left(-\frac{4|\xi|^2\tau k}{\pi^2\epsilon}\right),
\end{aligned}$$

for $|\xi|>\frac{1}{\epsilon}$, which implies that (IV) satisfies the inequality

$$\begin{aligned}
(IV) &\leq \frac{4\ \tau k\ h^2}{6\epsilon}\int_0^{\frac{\sqrt{2}\pi}{h}}\int_0^{\frac{\pi}{2}}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}(r^2+z^2)^2\ \exp\left(-\frac{4(r^2+z^2)\tau k}{\pi^2\epsilon}\right)rdzd\varphi dr\\
&\leq \frac{\pi}{3\epsilon^{\frac{3}{2}}\ h\ (\tau k)^{\frac{3}{2}}}\ A(h,\tau,\epsilon,k),
\end{aligned}$$

where

$$\begin{aligned}
A(h,\tau,\epsilon,k) = \ & -\tfrac{\epsilon\pi^{\frac{7}{2}}}{128\ \tau k\ h}\left\{-\epsilon^2\pi^4h^4+\left[\epsilon^2\pi^4h^4+8\epsilon\pi^4\tau kh^2+32\tau^2k^2\pi^4\right]\exp\left(-\tfrac{8\tau k}{h^2\epsilon}\right)\right\}\\
&+\tfrac{\epsilon^{\frac{3}{2}}\pi^4}{64(\tau k)^{\frac{1}{2}}}\left\{-\epsilon\pi^2h^2\exp\left(-\tfrac{4\tau k}{h^2\epsilon}\right)+\left[\epsilon h^2\pi^2+8\pi^2\tau k\right]\exp\left(-\tfrac{12\tau k}{\epsilon h^2}\right)\right\}\\
&-\tfrac{\epsilon^2\pi^{\frac{11}{2}}h}{256\tau k}\left\{-\epsilon h^2\pi^2+\left[\epsilon h^2\pi^2+8\pi^2\tau k\right]\exp\left(-\tfrac{8\tau k}{h^2\epsilon}\right)\right\}\\
&-\tfrac{(\epsilon\tau k)^{\frac{1}{2}}\pi^7}{32}\left\{\exp\left(-\tfrac{4\tau k}{h^2\epsilon}\right)-\exp\left(-\tfrac{12\tau k}{h^2\epsilon}\right)\right\}\\
&-\tfrac{3\epsilon^{\frac{5}{2}}\pi^7h^2}{256(\tau k)^{\frac{1}{2}}}\left\{\exp\left(-\tfrac{4\tau k}{h^2\epsilon}\right)-\exp\left(-\tfrac{12\tau k}{h^2\epsilon}\right)\right\}\\
&+\tfrac{3\epsilon^3\pi^{\frac{15}{2}}h^3}{\tau k}\left\{1-\exp\left(-\tfrac{8\tau k}{h^2\epsilon}\right)\right\}.
\end{aligned}$$

Let us now study the term (III). We use again the moduli inequality in order to obtain

$$\left|2\tau k\epsilon^{\frac{1}{2}}\ (1-i\tau d^2)^{k-1}-\exp\left(-\frac{\left|d+\frac{1}{\epsilon}\right|^2\tau k}{\epsilon}\right)\right| \leq 2\tau k\epsilon^{\frac{1}{2}}\ \left|1-i\tau d^2\right|^{k-1}+\exp\left(-\frac{\left|d+\frac{1}{\epsilon}\right|^2\tau k}{\epsilon}\right). \tag{4.32}$$

Since $|1-i\tau d^2|\leq\sqrt{1+\tau^2d^4}\leq 1+\tau^2d^4$ we obtain

$$(4.32)\leq \underbrace{2\tau k\epsilon^{\frac{1}{2}}\ (1+\tau^2d^4)^{k-1}}_{(V)}+\underbrace{\exp\left(-\frac{d^2\tau k}{\epsilon}\right)}_{(VI)}. \tag{4.33}$$

On one hand, taking into account the following relation for positive real numbers

$$\left(1+\frac{1}{x}\right)^{x} < e < \left(1+\frac{1}{x}\right)^{x+1}, \tag{4.34}$$

we have

$$\begin{aligned}(V) = 2\tau k\epsilon^{\frac{1}{2}}(1+\tau^2 d^4)^{k-1} < 2\tau k\epsilon^{\frac{1}{2}}\exp\left(\tau^2 d^4\right) &< 2\tau k\epsilon^{\frac{1}{2}}(1+\tau^2 d^4)^{k+\tau^2 d^4} \\ &\leq 2\tau k\epsilon^{\frac{1}{2}}(1+\tau^2 d^4)^{k+\tau^2|\xi|^4},\end{aligned}$$

since $\tau^2 < \frac{h^4}{64}$. Moreover, the following refinement is valid

$$\begin{aligned}\tau^2 d^4 < d^4\frac{h^4}{64} &= \frac{h^4}{64}\frac{256}{h^4}\left(\sin^2\left(\frac{h\xi_1}{2}\right)+\sin^2\left(\frac{h\xi_2}{2}\right)+\sin^2\left(\frac{h\xi_3}{2}\right)\right)^2 \\ &\leq 4(1+1+1)^2 \\ &= 36.\end{aligned}$$

For the second term (and assuming $d > 0$), since we have

$$\left|\xi-\frac{\vec{1}}{\epsilon}\right|^2-\left|d-\frac{1}{\epsilon}\right|^2 \leq \frac{h^2}{12}\left|\xi-\frac{\vec{1}}{\epsilon}\right|^2$$

that is

$$-\left|d-\frac{1}{\epsilon}\right|^2 \leq \left(\frac{h^2}{12}-1\right)\left|\xi-\frac{\vec{1}}{\epsilon}\right|^2 < 0$$

whenever $h < \sqrt{12}$. Hence,

$$\left|d-\frac{1}{\epsilon}\right|^2 \geq \left(1-\frac{h^2}{12}\right)\left|\xi-\frac{\vec{1}}{\epsilon}\right|^2 \geq \left(1-\frac{h^2}{12}\right)\left(|\xi|^2+\frac{1}{\epsilon^2}\right)$$

and from $\left|d-\frac{1}{\epsilon}\right|^2 \leq d^2 \leq \left|d+\frac{1}{\epsilon}\right|^2$ we can conclude that

$$(VI) \leq \exp\left(-\frac{|d-\frac{1}{\epsilon}|^2\tau k}{\epsilon}\right) \leq \exp\left(-\frac{\tau k}{\epsilon}\left(1-\frac{h^2}{12}\right)\left(|\xi|^2+\frac{1}{\epsilon^2}\right)\right).$$

Therefore, we have

$$
\begin{aligned}
(III) \quad \leq \quad & 2\tau k\epsilon^{\frac{1}{2}} \left|\left|36^{k-1+\tau^2|\xi|^4}\right|\right|_{L_1(Q_h)} + \left|\left|\exp\left(-\frac{\tau k}{\epsilon}\left(1-\frac{h^2}{2}\right)\left(|\xi|^2-\frac{1}{\epsilon^2}\right)\right)\right|\right|_{L_1(Q_h)} \\
\leq \quad & 8\tau k\epsilon^{\frac{1}{2}} \int_0^{\frac{\sqrt{2}\pi}{h}} \int_0^{\frac{\pi}{2}} \int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} 36^{k-1+\tau^2(r^2+z^2)^2} r dz\ d\varphi\ dr \\
& +4 \int_0^{\frac{\sqrt{2}\pi}{h}} \int_0^{\frac{\pi}{2}} \int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} \exp\left(-\frac{\tau k}{\epsilon}\left(1-\frac{h^2}{2}\right)\left(|\xi|^2-\frac{1}{\epsilon^2}\right)\right) r dz d\varphi dr \\
= \quad & \frac{\epsilon^{\frac{3}{2}}(2\pi)^{\frac{1}{2}}}{(\tau k(2-h^2))^{\frac{3}{2}}} \exp\left(-\frac{\tau k(-2h^2+h^4+4\epsilon^2\pi^2)}{(h\epsilon)^2}\right)\left(\exp\left(-\frac{\tau k\pi^2}{\epsilon}\right)-\exp\left(-\frac{2\tau k\pi^2}{\epsilon h^2}\right)\right).
\end{aligned}
$$

Combining the estimates obtained for (III) and (IV), we finally conclude that

$$
\begin{aligned}
(4.31) \leq & \frac{H(\tau k)}{(2\pi)^{\frac{3}{2}}\ 2\ \tau k\ \epsilon^{\frac{1}{2}}} \left\{ \frac{\pi}{3\epsilon^{\frac{3}{2}}\ h\ (\tau k)^{\frac{3}{2}}}\ A(h,\tau,\epsilon,k) \right. \\
& \left. + \frac{\epsilon^{\frac{3}{2}}(2\pi)^{\frac{1}{2}}}{(\tau k(2-h^2))^{\frac{3}{2}}} \exp\left(-\frac{\tau k(-2h^2+h^4+4\epsilon^2\pi^2)}{(h\epsilon)^2}\right)\left(\exp\left(-\frac{\tau k\pi^2}{\epsilon}\right)-\exp\left(-\frac{2\tau k\pi^2}{\epsilon h^2}\right)\right)\right\}.
\end{aligned} \tag{4.35}
$$

Then, by (4.30) e (4.35) we get

$$
\begin{aligned}
& ||e_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h)} \leq M(\epsilon,k,h,\tau) := \\
:= & Vol(G_h) \max_{h\underline{m}\in G_h} \left\{ \frac{H(\tau k)\ \epsilon^{\frac{5}{2}}}{(2\pi)^{\frac{3}{2}}(\tau k)^{\frac{7}{2}}}\ \exp\left(-\frac{\tau k\pi^2}{h^2\epsilon}\right) + \frac{\pi}{3\epsilon^{\frac{3}{2}}\ h\ (\tau k)^{\frac{3}{2}}}\ A(h,\tau,\epsilon,k) \right. \\
& \left. + \frac{\epsilon^{\frac{3}{2}}(2\pi)^{\frac{1}{2}}}{(\tau k(2-h^2))^{\frac{3}{2}}} \exp\left(-\frac{\tau k(-2h^2+h^4+4\epsilon^2\pi^2)}{(h\epsilon)^2}\right)\left(\exp\left(-\frac{\tau k\pi^2}{\epsilon}\right)-\exp\left(-\frac{2\tau k\pi^2}{\epsilon h^2}\right)\right)\right\},
\end{aligned} \tag{4.36}
$$

for $\epsilon > 0$.

Finally, adding (4.36) with respect to the time-lattice we obtain an estimate for the l_1-norm in the lattice $G_h \times (T_0,+\infty)_\tau$,

$$
\begin{aligned}
||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h\times(T_0,+\infty)_\tau)} &= \Big|\Big|\ ||e_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h)}\Big|\Big|_{l_1((T_0,+\infty)_\tau)} \\
&= \sum_{k=k_0+1}^{+\infty} \tau||e_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h)} \\
&\leq \sum_{k=k_0+1}^{+\infty} \tau M(\epsilon,k,h,\tau).
\end{aligned} \tag{4.37}
$$

Now, by the ratio test for real series of positives terms, we conclude that the previous series is convergent, since $\tau^2 < \frac{h^4}{64}$ and its sum, which we will denote by $S_M(\epsilon,h,\tau)$, tends to zero when $\epsilon, h, \tau \to 0$. Moreover, next we will proof the existence of $T_0 > 0$ such that both (4.26) and (4.37) are positive.

Main Result

Using inequalities (4.26) and (4.37) we obtain the general estimation

$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}_\tau^+)} \leq T_0 + T_0\ C_1(h) + T_0\ C_2(h, k_0) + S_M(\epsilon, h, \tau). \tag{4.38}$$

For the purpose of convergence we require that $h \leq h_0$, where h_0 is constant. In the following convergence theorem we prove the existence of $T_0 > 0$ for which (4.38) is positive always.

Theorem 4.3.1 *Let $\tau^2 < \frac{h^4}{64}$. Then there is a valid the convergence*

$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}_\tau^+)} \to 0,$$

when $h, \tau, \epsilon \to 0$.

Proof: We prove that for arbitrary $\delta > 0$ there exists a constant $h^* > 0$ such that for all $h < \min\{h^*, h_0\}$ and for all $\tau^2 < \frac{h^4}{64}$ it follows

$$||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}_\tau^+)} \leq \delta.$$

We choose

$$T_0 = \frac{\left(\sqrt{\frac{h_0^2}{\pi} + \frac{\delta}{4}\left(2 + \frac{C_1(h_0)}{4\pi}\right)} - \frac{h_0}{\sqrt{\pi}}\right)^2}{\left(2 + \frac{C_1(h_0)}{4\pi}\right)^2} > 0$$

and

$$h^* = \min\left\{\sqrt{\frac{T_0\delta}{4}}, \sqrt{\frac{3\pi^2 T_0}{2}}\right\}.$$

We remark that T_0 is not necessary a point of the lattice $\mathbb{R}_\tau^+$. We rectify this quantity by

$$T_0^+ = T_0 + \alpha\tau \qquad \text{and} \qquad T_0^- = T_0 - (1-\alpha)\tau,$$

with $\alpha \in [0, 1[$ such that $T_0^+, T_0^- \in \mathbb{R}_\tau^+$. We have then

$$\begin{aligned} ||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}_\tau^+)} \quad &\leq \quad ||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]0, T_0^+]_\tau)} \\ &\quad + ||e_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times (T_0^-, +\infty))}. \end{aligned}$$

A simple estimation using (4.26) and (4.37) shows that the right hand side of the last inequality is bounded by δ.

■

Implicit case

In this section we construct a fundamental solution $e^*_{h,+\tau}$ for the implicit equation

$$(-\Delta_h e^*_{h,+\tau})(h\underline{m}, \tau(k+1)) - i(\partial_\tau e^*_{h,+\tau})(h\underline{m}, \tau k) = \delta_h(h\underline{m})\ \delta_\tau(\tau k), \tag{4.39}$$

and we establish convergent results in a similar way as done in the Subsubsection 4.3.1.

Applying the discrete Fourier transform we obtain

$$(\mathcal{F}_h e^*_{h,+\tau})(\xi, t) = \frac{i}{2\pi}\ \left(1 + i\tau d^2\right)^{-\frac{t}{\tau}} \chi_h(\xi),$$

in analogy to Section 4.3.1. From this, we get the following system of equations which allow us to calculate $e^*_{h,+\tau}$

$$\left\{\begin{array}{c} e^*_{h,+\tau}(h\underline{m}, 0) = 0 \\ ((1 - i\tau\Delta_h)e^*_{h,+\tau})(h\underline{m}, \tau) = \delta_h(h\underline{m}) \\ ((1 - i\tau\Delta_h)e^*_{h,+\tau})(h\underline{m}, \tau(k+1)) = e^*_{h,+\tau}(h\underline{m}, \tau k) \end{array}\right. , \tag{4.40}$$

where $k \in \mathbb{Z}^+$ and $\underline{m} \in \mathbb{Z}^3$. We remark that it is also possible to describe the fundamental solution by applying $\mathcal{F}^{-1} = R_h\mathcal{F}$, that is

$$e^*_{h,+\tau}(h\underline{m}, \tau k) = R_h\mathcal{F}\left(\frac{H(t)}{2\pi}(1 + i\tau d^2)^{-k}\chi_h(\xi)\right)(h\underline{m}, \tau k).$$

However, this does not prove our assertion, that of $e^*_{h,+\tau}$ being a fundamental solution for the operator in (4.17).

Existence of Fundamental Solution

For the proof of the existence we require the following two lemmas. Their proofs can be found in [38] and, therefore, will be omitted here.

Lemma 4.3.2 *Let f_h be an arbitrary bounded function in $\mathbb{R}^3_h$. Then the equation*

$$(1 - i\tau\Delta_h)v_h = f_h,$$

has a unique solution v_h in $\mathbb{R}^3_h$.

Lemma 4.3.3 *If $f_h \in l_1(\mathbb{R}_h^3)$, then $v_h \in l_1(\mathbb{R}_h^3)$.*

With the help of these two results we can present the following theorem.

Theorem 4.3.4 *System (4.40) has an unique solution $e^*_{h,+\tau}$. Moreover, for an arbitrary finite $T_0 > 0$ it holds $e^*_{h,+\tau} \in l_1(\mathbb{R}_h^3 \times]0, T_0])$.*

Proof: The first assertion follows directly from Lemmas 4.3.2 and 4.3.3. Indeed, Lemma 4.3.2 ensures the existence and uniqueness of $e^*_{h,+\tau}$ while Lemma 4.3.3 guarantees that for each fixed time-step the fundamental solution is an element of $l_1(\mathbb{R}_h^3)$. The second assertion is an obvious consequence of $e^*_{h,+\tau}(\cdot, \tau k) \in l_1(\mathbb{R}_h^3)$.

∎

Convergence

We now investigate the l_1-convergence of our solution $e^*_{h,+\tau}$ to $R_\tau R_h e_+$ in the lattice $G_h \times \mathbb{R}_\tau^+$.

Again we divide this study into the cases of a finite time interval $]0, T_0]_\tau$ and its unbounded complement $(T_0, \infty)_\tau$, where $T_0 = \tau k_0$, $k_0 \in \mathbb{N}$. For the first case, we use the discrete Laplacian in order to write the second difference equation on system (4.40) as

$$\left(1 + i\frac{6\tau}{h^2}\right) e^*_{h,+\tau}(h\underline{m}, \tau) = \delta_h(h\underline{m}) - i\frac{\tau}{h^2}\sum_{j=1}^{3}\left[e^*_{h,+\tau}(h\underline{m} \pm m_j e_j, \tau)\right]$$

and we obtain for the l_1-norm of $e^*_{h,+\tau}(\cdot, \tau)$ the inequality (after re-arrangement of the sum's indexes)

$$\left|1 + i\frac{6\tau}{h^2}\right| \sum_{\underline{m}\in\mathbb{R}_h^3} \left|e^*_{h,+\tau}(h\underline{m}, \tau)\right| h^3 \quad \leq \quad 1 + \frac{6\tau}{h^2}\sum_{\underline{m}\in\mathbb{R}_h^3}\left|e^*_{h,+\tau}(h\underline{m}, \tau)\right| h^3,$$

which in its turn implies that

$$||e^*_{h,+\tau}(\cdot, \tau)||_{l_1(\mathbb{R}_h^3)} \leq 1.$$

In the same way we prove the inequality

$$||e^*_{h,+\tau}(\cdot, \tau(k+1))||_{l_1(\mathbb{R}_h^3)} \leq ||e^*_{h,+\tau}(\cdot, \tau k)||_{l_1(\mathbb{R}_h^3)},$$

for $k \geq 1$. Then,

$$||e^*_{h,+\tau}||_{l_1(G_h \times]0,T_0]_\tau)} \leq ||e^*_{h,+\tau}||_{l_1(\mathbb{R}_h^3 \times]0,T_0]_\tau)} \leq \sum_{k=1}^{k_0} \tau = T_0.$$

Moreover, using the l_1- norm of the space-time-discretization for the continuous fundamental solution (estimate as in (4.25)) we get for $||e^*_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]0,T_0]_\tau)}$ the same estimate as in (4.26).

As done previously for the case of the interval unbounded in time $(T_0,\infty)_\tau$ we use the family of regularized solutions (4.27) and, therefore,

$$||e^*_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h)} \leq$$
$$||R_\tau R_h(e^\epsilon_+(\cdot,\tau k) - e_+(\cdot,\tau k))||_{l_1(G_h)} + ||e^*_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e^\epsilon_+(\cdot,\tau k)||_{l_1(G_h)}. \tag{4.41}$$

Again, it will be enough to construct an estimate for the last term of this inequality. As in (4.28) the behavior of the second term depends on

$$\begin{aligned} ||(\mathcal{F}_h e^*_{h,+\tau})(\cdot,\tau k) - (R_\tau \mathcal{F}^{-1} e^\epsilon_+)(\cdot,\tau k)||_{L_1(\mathbb{R}^3)} \leq & \underbrace{||(\mathcal{F}_h e^*_{h,+\tau})(\cdot,\tau k) - (R_\tau \mathcal{F}^{-1} e^\epsilon_+)(\cdot,\tau k)||_{L_1(\mathbb{R}^3\setminus Q_h)}}_{(VII)} \\ & + \underbrace{||(\mathcal{F}_h e^*_{h,+\tau})(\cdot,\tau k) - (R_\tau \mathcal{F}^{-1} e^\epsilon_+)(\cdot,\tau k)||_{L_1(Q_h)}}_{(VIII)} \end{aligned}$$

Let us now study (VII). Taking into account the properties of the discrete Fourier transform and the calculations for (4.30) we conclude

$$(VII) \leq \frac{H(\tau k)}{(2\pi)^{\frac{3}{2}}(\tau k)^{\frac{3}{2}}} \exp\left(-\frac{\tau k \pi^2}{h^2 \epsilon}\right).$$

Taking into account (4.31), we have for the remaining term $(VIII)$ the estimative

$$\begin{aligned} (VIII) &= \frac{H(\tau k)}{2\tau k (2\pi)^{\frac{3}{2}} \epsilon^{\frac{1}{2}}} \left\| 2\tau k \epsilon^{\frac{1}{2}} (1 + i\tau d^2)^{-k} - \exp\left(-\frac{\left|\xi + \frac{\vec{1}}{\epsilon}\right|^2 \tau k}{\epsilon}\right) \right\|_{L_1(Q_h)} \\ &\leq \frac{H(\tau k)}{2\tau k (2\pi)^{\frac{3}{2}} \epsilon^{\frac{1}{2}}} \left\{ \underbrace{\left\| 2\tau k \epsilon^{\frac{1}{2}} (1 + i\tau d^2)^{-k} - \exp\left(-\frac{\left|d + \frac{1}{\epsilon}\right|^2 \tau k}{\epsilon}\right) \right\|_{L_1(Q_h)}}_{(IX)} \right. \\ & \left. + \underbrace{\left\| \exp\left(-\frac{\left|d + \frac{1}{\epsilon}\right|^2 \tau k}{\epsilon}\right) - \exp\left(-\frac{\left|\xi + \frac{\vec{1}}{\epsilon}\right|^2 \tau k}{\epsilon}\right) \right\|_{L_1(Q_h)}}_{(X)} \right\} \end{aligned} \tag{4.42}$$

As we can see $(X) = (IV)$, which implies that we need to study only (IX). We have the following relation

$$\left|2\tau k\epsilon^{\frac{1}{2}}(1+i\tau d^2)^{-k} - \exp\left(-\frac{\left|d+\frac{1}{\epsilon}\right|^2\tau k}{\epsilon}\right)\right| \leq 2\tau k\epsilon^{\frac{1}{2}}\left|1+i\tau d^2\right|^{-k} + \exp\left(-\frac{\left|d+\frac{1}{\epsilon}\right|^2\tau k}{\epsilon}\right) \quad (4.43)$$

Since $|1-i\tau d^2| \geq |1-i\tau d| = \sqrt{1+\tau^2 d^2}$, we conclude

$$(4.43) \leq \underbrace{2k\tau\epsilon^{\frac{1}{2}}(1+\tau^2 d^2)^{-\frac{k}{2}}}_{(XI)} + \underbrace{\exp\left(-\frac{d^2\tau k}{\epsilon}\right)}_{(XII)}.$$

Again, $(XII) = (VI)$, which implies that we need to study only (XI). Taking into account (4.34), we have

$$\begin{aligned} 2\tau k\epsilon^{\frac{1}{2}}(1+\tau^2 d^4)^{-\frac{k}{2}} < 2\tau k\epsilon^{\frac{1}{2}}\exp\left(\tau^2 d^2\right) & < 2\tau k\epsilon^{\frac{1}{2}}(1+\tau^2 d^2)^{-\frac{k}{2}+1+\tau^2 d^2} \\ & < 2\tau k\epsilon^{\frac{1}{2}}(1+\tau^2 d^2)^{-\frac{k}{2}+1+\tau^2|\xi|^2}, \end{aligned}$$

since $\tau^2 < \frac{h^2}{64}$.

Moreover, it holds

$$\begin{aligned} \tau^2 d^2 < d^2\frac{h^2}{64} &= \frac{h^2}{64}\,\frac{16}{h^2}\left(\sin^2\left(\frac{h\xi_1}{2}\right)+\sin^2\left(\frac{h\xi_2}{2}\right)+\sin^2\left(\frac{h\xi_3}{2}\right)\right)^2 \\ &\leq \frac{1}{4}(1+1+1)^2 \\ &= \frac{3}{4}. \end{aligned}$$

Then we have

$$\begin{aligned} \left|\left|2k\tau\epsilon^{\frac{1}{2}}(1+i\tau d^2)^{-k}\right|\right|_{L_1(Q_h)} &\leq 2k\tau\epsilon^{\frac{1}{2}}\left|\left|\left(\frac{3}{4}\right)^{-\frac{k}{2}+1+\tau^2|\xi|^2}\right|\right|_{L_1(Q_h)} \\ &= 8k\tau\epsilon^{\frac{1}{2}}\int_0^{\frac{\sqrt{2}\pi}{h}}\int_0^{\frac{\pi}{2}}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}\left(\frac{3}{4}\right)^{-\frac{k}{2}+1+\tau^2(r^2+z^2)^2} r\,dz\,d\varphi\,dr \\ &= C_k\tau\epsilon^{\frac{1}{2}}, \end{aligned}$$

where $C_k\tau\epsilon^{\frac{1}{2}} \to 0$, as $\epsilon \to 0$.

For (4.43) we obtain the same estimation as in (4.36). In the same way for $||e^*_{h,+\tau}(\cdot,\tau k) - R_\tau R_h e_+(\cdot,\tau k)||_{l_1(G_h\times\mathbb{R}^+_\tau)}$ we have the same estimation as in (4.38). Moreover, an analogue of Theorem 4.3.1 (Convergence Theorem) is also valid in this case.

Theorem 4.3.5 *For $h, \tau, \epsilon \to 0$ we have the convergence*

$$||e^*_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}^+_\tau)} \to 0,$$

when $\tau^2 < \frac{d^2}{64}$.

Proof: We have to show that for arbitrary $\delta > 0$ there exists $h^* > 0$ and $\tau > 0$ such that for all $h < \min(h^*, h_0)$ and $\tau < \tau^*$ it follows

$$||e^*_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times \mathbb{R}^+_\tau)} < \delta.$$

We take T_0 as in the proof of Theorem 4.3.1, and

$$\tau^* = \frac{T_0}{2} \qquad \text{and} \qquad h^* = \sqrt{\frac{\delta T_0}{8}}.$$

Using the estimation of $||e^*_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]0,T_0]_\tau)}$ for $T_0^+ = T_0 + \alpha\tau$ and the estimation of $||e^*_{h,+\tau} - R_\tau R_h e_+||_{l_1(G_h \times]T_0,+\infty[_\tau)}$ for $T_0^- = T_0 - (1-\alpha)\tau$ with $\alpha \in [0,1[$ such that $T_0^+,\ T_0^- \in \mathbb{R}^+_\tau$, we obtain the desired result.

■

Corollary 4.3.6 *Under the conditions of the previous theorem it holds*

$$||E_{h,+\tau} - E_+||_{l_1(G_h \times [0,+\infty)_\tau)} \to 0$$

for any bounded discrete domain $G_h \subset \mathbb{R}^3$, as $h, \tau \to 0$.

While we can prove the convergence of the discrete fundamental solution $e_{h,+\tau}$ to e_+, the proofs do not yield the order of convergence due to the natura of the continuous fundamental solution of the Schrödinger equation. This will be the subject of future work.

4.3.2 Discrete operators

Taking into account the conclusions regarding the discrete fundamental solution, we can establish the discrete analogue of the Teodorescu operator

Theorem 4.3.7 *For all $u \in l_p(\Omega_{h,\tau})$, $1 < p < +\infty$, such that $u : \Omega_{h,\tau} \to \mathbb{C}^4$ we have the discrete Teodorescu operator $T_{h,-\tau}$ satisfying to*

$$D_{h,-\tau}T_{h,-\tau}u(h\underline{m}, k\tau) = u(h\underline{m}, k\tau), \tag{4.44}$$

where

$$T_{h,-\tau}u(h\underline{m}, k\tau) = -\sum_{(h\underline{n},s\tau)\in\ \Omega_{h,\tau}} h^3\tau E_{h,+\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)u(h\underline{n}, s\tau), \tag{4.45}$$

for all $(h\underline{m}, k\tau) \in \Omega_{h,\tau}$.

Proof: We have for $T_{h,-\tau}$ that

$$D_{h,-\tau}T_{h,-\tau}u(h\underline{m}, k\tau) = \sum_{(h\underline{n},s\tau)\in\ \Omega_{h,\tau}} h^3\tau[D_{h,-\tau}E_{h,+\tau}](h\underline{m} - h\underline{n}, k\tau - s\tau)u(h\underline{n}, s\tau).$$

Since $E_{h,+\tau} = e_{h,+\tau}D_{h,+\tau}$ and $e_{h,+\tau}$ is a scalar solution, we have

$$\begin{aligned} D_{h,-\tau}T_{h,-\tau}u(h\underline{m}, k\tau) &= \sum_{(h\underline{n},s\tau)\in\ \Omega_{h,\tau}} h^3\tau[e_{h,+\tau}(D_{h,+\tau})^2(h\underline{m} - h\underline{n}, k\tau - s\tau)]u(h\underline{n}, s\tau) \\ &= \sum_{(h\underline{n},s\tau)\in\ \Omega_{h,\tau}} h^3\tau\ [\delta_h(h\underline{m} - h\underline{n})\delta_\tau(k\tau - s\tau)u(h\underline{n}, s\tau)] \\ &= u(h\underline{m}, k\tau). \end{aligned}$$

■

Now we are able to present the following norm estimate.

Theorem 4.3.8 *For all $u \in l_p(\Omega_{h,\tau})$, $1 < p < +\infty$, such that $u : \Omega_{h,\tau} \to \mathbb{C}^4$ there exists a positive constant $C > 0$ such that*

$$||T_{h,-\tau}u||_{l_p(\Omega_{h,\tau})} \leq C||u||_{l_p(\Omega_{h,\tau})}.$$

Moreover, $T_{h,-\tau}$ is a continuous operator.

Proof: Initially we have

$$\begin{aligned} ||T_{h,-\tau}u||_{l_p(\Omega_{h,\tau})} &= \left(\sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau}} \tau h^3\,|E_{h,+\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)u(h\underline{n}, s\tau)|^p\right)^{\frac{1}{p}} \\ &\leq \left(\sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau}} \tau h^3\,|E_{h,+\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)|^p\,|u(h\underline{n}, s\tau)|^p\right)^{\frac{1}{p}}. \end{aligned}$$

Let us take $C(\underline{m},k) = \max_{(h\underline{n},s\tau)\in\Omega_{h,\tau}} |E_{h,+\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)|$. Then there exists $C = \max C(\underline{m},k) > 0$, this maximum being taken over all $(\underline{m},k)$ such that $(h\underline{m},k\tau) \in \Omega_{h,\tau}$, and the result holds.

■

As we have done for the analytic case we can establish a decomposition of the l_p-space.

Theorem 4.3.9 *For the space $l_p(\Omega_{h,\tau})$, $1 < p < \infty$, the following direct decomposition*

$$l_p(\Omega_{h,\tau}) = \ker D_{h,-\tau}(\mathrm{int}\Omega_{h,\tau}) \oplus D_{h,-\tau}(\overset{\circ}{w}{}_p^1(\Omega_{h,\tau}))$$

is valid, with correspondent discrete projection operators

$$P_{h,-\tau} : l_p(\Omega_{h,\tau}) \mapsto \ker D_{h,-\tau}(\mathrm{int}\Omega_{h,\tau}),$$
$$Q_{h,-\tau} : l_p(\Omega_{h,\tau}) \mapsto D_{h,-\tau}(\overset{\circ}{w}{}_p^1(\Omega_{h,\tau})),$$

where $\overset{\circ}{w}{}_p^1(\Omega_{h,\tau})$ denotes the discrete counterpart of the Sobolev space $\overset{\circ}{W}{}_p^1(\Omega)$.

The proof of this result is equivalent to the proof presented for the analytic case (Chapter 3).

Remark 4.3.10 *A similar decomposition result can be obtained for the operator $D_{h,-\tau}$.*

We say that $u \in C^{1,\alpha}(\Omega)$ if its first derivatives are α-Hölder continuous.

Theorem 4.3.11 *Let $u \in C^{1,\alpha}(\Omega)$. Then it holds $T_{h,-\tau}u \to Tu$ as h, τ tend to zero.*

Proof: As it was done in Chapter 3 during the application of the regularization procedure, we construct the regularized discrete Teodorescu operator $T^{\epsilon}_{h,-\tau}$ in terms of the regularized discrete fundamental solution (4.19).

By definition, we have

$$|T^{\epsilon}_{h,-\tau}u(h\underline{m},k\tau) - T^{\epsilon}u(h\underline{m},k\tau)| \leq \left| \sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau}} E^{\epsilon}_{h,+\tau}(h\underline{m} - h\underline{n}, k\tau - s\tau)u(h\underline{n},s\tau)h^3\tau \right.$$
$$\left. - \int_{\Omega} E^{\epsilon}_{+}(h\underline{m} - z, k\tau - r)u(z,r)dzdr \right|. \quad (4.46)$$

Because of the singularity of the continuous fundamental solution E^{ϵ}_{+}, we will split the continuous domain Ω into parallelepiped $W(h\underline{n},\tau s)$ centered at the points $(h\underline{n},\tau s)$ of the lattice $\Omega_{h,\tau}$ with side-lengths h and τ, respectively. Furthermore, let $p,q\in\mathbb{N}$ be such that $\frac{1}{p}+\frac{1}{q}=1$. We have then

$$
\begin{aligned}
(4.46) \quad \leq \quad & \sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau}} \left|[E^{\epsilon}_{h,+\tau}(h\underline{m}-h\underline{n},k\tau-s\tau)-E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)]u(h\underline{n},s\tau)h^3\tau\right| \\
& + \left| \sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau}} \left[E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)u(h\underline{n},s\tau)h^3\tau \right.\right. \\
& \left.\left. - \int_{W(h\underline{n},s\tau)} E^{\epsilon}_{+}(h\underline{m}-z,k\tau-r)u(z,r)dzdr \ \right]\right|. \qquad (4.47)
\end{aligned}
$$

We use Hölder inequality on the first term and by a convenient adding up we get

$$
\begin{aligned}
(4.47) \quad \leq \quad & ||E^{\epsilon}_{h,+\tau}-E^{\epsilon}_{+}||_{l_p(\Omega_{h,\tau})}||u||_{l_q(\Omega_{h,\tau})} \\
& + \underbrace{\sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau},\ z\in W(h\underline{n},s\tau)} \left[\left| \ E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)[u(h\underline{n},s\tau)-u(z,r)]h^3\tau\right|\right.}_{(I_1)} \\
& + \underbrace{\int_{W(h\underline{n},s\tau)} \left|\left[E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)-E^{\epsilon}_{+}(h\underline{m}-z,k\tau-r)\right]u(z,r)\right|dzdr \ \Big].}_{(I_2(h\underline{n},s\tau))}
\end{aligned}
$$

For the term (I_1) we obtain

$$
\begin{aligned}
(I_1) \quad \leq \quad & \sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau},\ z\in W(h\underline{n},s\tau)} |E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)| \int_{W(h\underline{n},s\tau)} |u(h\underline{n},s\tau)-u(z,r)|dzdr \\
\leq \quad & \sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau},\ z\in W(h\underline{n},s\tau)} |E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)| C \int_{W(h\underline{n},s\tau)} |(h\underline{n}-z,s\tau-r)|^{\alpha}dzdr,
\end{aligned}
$$

which goes to zero as $h,\tau\to 0$.

Finally the term $(I_2(h\underline{n},s\tau))$ can be estimate using its Taylor series expansion and Hölder's inequality

$$
\begin{aligned}
(I_2(h\underline{n},s\tau)) \quad \leq \quad & \int_{W(h\underline{n},s\tau)} \left|\left[E^{\epsilon}_{+}(h\underline{m}-h\underline{n},k\tau-s\tau)-E^{\epsilon}_{+}(h\underline{m}-z,k\tau-r)\right]u(z,r)\right|dzdr \\
\leq \quad & \int_{W(h\underline{n},s\tau)} \left|\nabla E^{\epsilon}_{+}(h\underline{m}-z,k\tau-r)\cdot(h\underline{n}-z,s\tau-r)\right| |u(z,r)|dzdr \\
\leq \quad & ||\nabla E^{\epsilon}_{+}(h\underline{m}-\cdot,k\tau-\cdot)\cdot(h\underline{n}-\cdot,s\tau-\cdot)||_{L_q(W(h\underline{n},s\tau))}||u||_{L_p(W(h\underline{n},s\tau))},
\end{aligned}
$$

and again we have that $\sum_{(h\underline{n},s\tau)\in\Omega_{h,\tau},\ z\in W(h\underline{n},s\tau)}(I_2(h\underline{n},s\tau))$ goes to zero as $h,\tau\to 0$.

Hence, by $\epsilon\to 0$ we obtain convergence of the discrete Teodorescu operator $T_{h,-\tau}$ to the continuous one.

■

Moreover, we notice that we have convergence in l_p, $1 < p < +\infty$, of the regularized discrete Teodorescu operator $T^{\epsilon}_{h,-\tau}$ to the regularized Teodorescu operator T^{ϵ}_{-}.

We now prove the convergence of the discrete Cauchy-Bitsadze operator $F_{h,-\tau} = I - T_{h,-\tau}D_{h,-\tau}$ to the Cauchy-Bitsadze operator.

Theorem 4.3.12 *If $u \in \ker D_-$ is such that $u \in C^{1,\alpha}(\Omega)$ for some $0 < \alpha < 1$ then we have*

$$||u - F_{h,-\tau}u||_{l_p(\Omega_{h,\tau})} \leq C||u||_{C^{1,\alpha}(\Omega)}(h^\alpha + \tau^\alpha),$$

for a positive constant $C > 0$.

Proof: We use the definition of $F_{h,-\tau}$, Theorem 4.3.8 and the fact that $u \in \ker(D_-)$. We get then

$$\begin{aligned}
||u - F_{h,-\tau}u||_{l_p(\Omega_{h,\tau})} &= ||T_{h,-\tau}D_{h,-\tau}u||_{l_p(\Omega_{h,\tau})} \\
&= ||T_{h,-\tau}(D_{h,-\tau}u - D_-u)||_{l_p(\Omega_{h,\tau})} \\
&\leq C_1||D_{h,-\tau}u - D_-u||_{l_p(\Omega_{h,\tau})} \\
&\leq C_1\left(||D_hu - Du||_{l_p(\Omega_{h,\tau})} + ||\partial_\tau u - \partial_t u||_{l_p(\Omega_{h,\tau})}\right) \\
&\leq C_1\left[\left(\sum_{(h\underline{m},k\tau)\in\Omega_{h,\tau}} |D_hu(h\underline{m},k\tau) - Du(h\underline{m},k\tau)|^p h^3\tau\right)^{\frac{1}{p}}\right. \\
&\quad \left. + \left(\sum_{(h\underline{m},k\tau)\in\Omega_{h,\tau}} |\partial_\tau u(h\underline{m},k\tau) - \partial_t u(h\underline{m},k\tau)|^p h^3\tau\right)^{\frac{1}{p}}\right]. \qquad (4.48)
\end{aligned}$$

Additionally, we remark that $u \in C^{1,\alpha}(\Omega)$ implies both that for each t fixed $u_0(\cdot,t) \in C^{1,\alpha}(\underline{\Omega})$, and for each x fixed $u_0(x,\cdot) \in C^{1,\alpha}([0,T))$.

Moreover, we have (c.f. [39], p. 268) that

$$|D_h^{+-}u(h\underline{m},k\tau) - Du(h\underline{m},k\tau)| \leq K(k\tau)||u(\cdot,k\tau)||_{C^{1,\alpha}(\Omega^{k\tau})}h^\alpha, \qquad (4.49)$$

a similar result holding D_h^{-+}, and

$$|\partial_\tau(h\underline{m},k\tau) - \partial_t u(h\underline{m},k\tau)| \leq K(h\underline{m})||u(h\underline{m},\cdot)||_{C^{1,\alpha}(\Omega^{h\underline{m}})}\tau^\alpha, \qquad (4.50)$$

for some positive constants $K(k\tau)$, $K(h\underline{m})$. Using these two inequalities we have

$$(4.48) \quad \leq \quad C_1 \left[\left(\sum_{(h\underline{m},k\tau)\in\Omega_{h,\tau}} K^p(k\tau)||u(\cdot,k\tau)||^p_{C^{1,\alpha}(\Omega^{k\tau})} h^{p\alpha}h^3\tau \right)^{1/p} + \left(\sum_{(h\underline{m},k\tau)\in\Omega_{h,\tau}} K^p(h\underline{m})||u(h\underline{m},\cdot)||^p_{C^{1,\alpha}(\Omega^{h\underline{m}})} \tau^{p\alpha}h^3\tau \right)^{1/p} \right].$$

We now take $K = \max_{\Omega_{h,\tau}}\{K(k\tau), K(h\underline{m})\} > 0$ and we recall that

$$||u(h\underline{m},\cdot)||_{C^{1,\alpha}(\Omega^{h\underline{m}})} \leq ||u||_{C^{1,\alpha}(\Omega)}, \quad ||u(\cdot,k\tau)||_{C^{1,\alpha}(\Omega^{k\tau})} \leq ||u||_{C^{1,\alpha}(\Omega)}.$$

Hence

$$(4.48) \leq C_1 K Vol(\Omega_{h,\tau})||u||_{C^{1,\alpha}(\Omega)}(h^\alpha + \tau^\alpha).$$

■

We are now in conditions to prove the convergence of the discrete projection operator $Q_{h,-\tau}$ to its continuous counterpart (see Theorem 3.2.32).

Theorem 4.3.13 *Let $u \in L_p(\Omega)$ for some $1 < p < \infty$. Then it holds for the projector $Q_{h,-\tau}$*

$$||Q_{h,-\tau}u - Q_-u||_{l_p(\Omega_{h,\tau})} \to 0 \quad as \quad h,\tau \ \to 0$$

for a positive constant C.

Proof: We start from the equality

$$\begin{aligned} Q_{h,-\tau}u - Q_-u &= Q_{h,-\tau}(P_-u + Q_-u) - Q_-(P_-u + Q_-u) \\ &= Q_{h,-\tau}P_-u + Q_{h,-\tau}Q_-u - Q_-u \end{aligned}$$

and we wish to obtain estimates for the terms $Q_{h,-\tau}P_-u$ and $(Q_{h,-\tau} - I)Q_-u$ (we recall that, being projection operators, $Q_-(P_-u) = 0$ and $Q_-^2 = Q_-$).

Since $P_-u = F_-P_-u$ and $Q_{h,-\tau}F_{h,-\tau}u = 0$, for the first term we obtain

$$\begin{aligned} Q_{h,-\tau}P_-u &= Q_{h,-\tau}F_-P_-u - Q_{h,-\tau}F_{h,-\tau}P_-u \\ &= Q_{h,-\tau}(F_- - F_{h,-\tau})P_-u \\ &= Q_{h,-\tau}(I - F_{h,-\tau} - T_-D_-)P_-u \\ &= Q_{h,-\tau}(I - F_{h,-\tau})P_-u \end{aligned}$$

and, therefore, by Theorem 4.3.12 we get the following estimate

$$\begin{aligned} ||Q_{h,-\tau}P_- u||_{l_p(\Omega_{h,\tau})} &\leq ||Q_{h,-\tau}||\ ||P_- u - F_{h,-\tau}P_- u||_{l_p(\Omega_{h,\tau})} \\ &\leq C||Q_{h,-\tau}||\ ||P_- u||_{C^{1,\alpha}(\Omega)}(h^\alpha + \tau^\alpha), \end{aligned}$$

taking in account that $Q_{h,-\tau}$ has bounded norm. Moreover, due to the fact that P_- is the projection into the kernel of $D_{h,-\tau}$, it holds $||P_- u||_{C^{1,\alpha}(\Omega)} < \infty$.

For the second term we remember that $Q_- u$ can be written as $Q_- u = D_- g$ where $g \in \overset{\circ}{W}{}_2^1(\Omega)$. This leads to

$$\begin{aligned} (Q_{h,-\tau} - I)Q_- u &= (Q_{h,-\tau} - I)D_- g \\ &= Q_{h,-\tau}(D_- g - D_{h,-\tau}g) + Q_{h,-\tau}D_{h,-\tau}g - D_- g \\ &= Q_{h,-\tau}(D_- g - D_{h,-\tau}g) + (D_{h,-\tau}g - D_- g), \end{aligned}$$

since $Q_{h,-\tau}D_{h,-\tau}g = D_{h,-\tau}g$. Hence, taking into account the previous calculations, Theorem 4.3.12 and relations (4.49) and (4.50) we finally obtain

$$||(Q_{h,-\tau} - I)Q_- u||_{l_p(\Omega_{h,\tau})} \leq (||Q_{h,-\tau}|| + 1)||D_{h,-\tau}g - D_- g||_{l_p(\Omega_{h,\tau})} \to 0$$

as h, τ goes to zero.

■

Remark 4.3.14 *In an analogous way we can prove the convergence of the projection operator $P_{h,-\tau}$ to its continuous counterpart (see Theorem 3.2.32).*

The above discrete operators allow us to establish a discrete equivalent of the Theorem 3.2.33.

Theorem 4.3.15 *Let $f \in l_2(\Omega_{h,\tau})$. The solution of the discrete Schrödinger problem*

$$\begin{cases} (-i\partial_\tau - \Delta_h)u = f \ \textit{in}\ \Omega_{h,\tau} \\ u = 0 \ \textit{on}\ \partial\Omega_{h,\tau} \end{cases}$$

is given by $u = -T_{h,-\tau}Q_{h,-\tau}T_{h,-\tau}f$.

4.3.3 Numerical examples

On the basis of the discrete operators previously introduced we construct the discrete version of problem (4.12) four our bonded domain

$$u = -T_{h,-\tau}Q_{h,-\tau}T_{h,-\tau}M(u) \text{ in } \Omega_{h,\tau}. \tag{4.51}$$

Indeed, let v be a solution of (4.51). Then

$$\begin{aligned}(-i\partial_\tau - \Delta_h)v &= D_{h,-\tau}D_{h,-\tau}[-T_{h,-\tau}Q_{h,-\tau}T_{h,-\tau}M(v)] \\ &= D_{h,-\tau}[Q_{h,-\tau}T_{h,-\tau}M(v)] \\ &= M(v),\end{aligned}$$

and due to the properties of the projector $Q_{h,-\tau}$ we have $v = 0$ on $\partial\Omega_{h,\tau}$.

Using the same ideas as in the continuous case (see [17]) we get results regarding the convergence and uniqueness of the discrete iterative method $u_{m+1} = -T_{h,-\tau}Q_{h,-\tau}T_{h,-\tau}M(u_m)$.

Theorem 4.3.16 *If $f \in l_2(\Omega_{h,\tau})$ then the discrete problem (4.51) has a unique solution $u \in \overset{\circ}{w}{}_2^1(\Omega_{h,\tau})$ whenever*

$$||f||_{l_2(\Omega_{h,\tau})} \leq \frac{1}{36C_{h,\tau}}$$

and the initial term $u_0 \in \overset{\circ}{w}{}_2^1(\Omega_{h,\tau})$ satisfies

$$||u_0||_{l_2(\Omega_{h,\tau})} \leq \frac{1}{6C_{h,\tau}} + W_{h,\tau},$$

with $W_{h,\tau} = \sqrt{\frac{1}{36C_{h,\tau}} - \frac{||f||_{l_2(\Omega_{h,\tau})}}{C_{h,\tau}}}$.

The proof of this theorem, being similar to the one in the continuous case, will be omitted.

The following results shows that the solution obtained for the discrete problem, which we will denote by u_*, converges to the solution obtained for the continuous, which we will denote by u. In the proof of the following theorem the restriction of $M(u)$ to the space-time grid will be denoted by $M_{h,\tau}(u)$.

Theorem 4.3.17 *Let $f \in L_2(\Omega)$. Then u_* converges to u in $\Omega_{h,\tau}$ whenever $h, \tau \to 0$.*

Proof: Again, we need to use the regularized Teodorescu operator. We shall denote $u_*^\epsilon = -T_{h,-\tau}^\epsilon Q_{h,-\tau} T_{h,-\tau}^\epsilon M_{h,\tau}(u_*^\epsilon)$ and $u^\epsilon = -T_-^\epsilon Q_- T_-^\epsilon M(u^\epsilon)$. We have

$$\begin{aligned}
||u_*^\epsilon - u^\epsilon||_{l_2(\Omega_{h,\tau})} &\leq \underbrace{||T_{h,-\tau}^\epsilon Q_{h,-\tau} T_{h,-\tau}^\epsilon M_{h,\tau}(u^\epsilon) - T_-^\epsilon Q_- T_-^\epsilon M(u^\epsilon)||_{l_2(\Omega_{h,\tau})}}_{(\mathbf{I})} \\
&\quad + ||T_{h,-\tau}^\epsilon Q_{h,-\tau} T_{h,-\tau}^\epsilon \left(M_{h,\tau}(u_*^\epsilon) - M_{h,\tau}(u^\epsilon)\right)||_{l_2(\Omega_{h,\tau})} \\
&\leq (\mathbf{I}) + C_{h,\tau} ||u_*^\epsilon - u^\epsilon||_{l_2(\Omega_{h,\tau})} \left(||u_*^\epsilon||_{l_2(\Omega_{h,\tau})} + ||u^\epsilon||_{l_2(\Omega_{h,\tau})} \right)
\end{aligned}$$

which implies that

$$||u_*^\epsilon - u^\epsilon||_{l_2(\Omega_{h,\tau})} \leq (\mathbf{I}) \left[1 - C_{h,\tau} \left(||u_*^\epsilon||_{l_2(\Omega_{h,\tau})} + ||u^\epsilon||_{l_2(\Omega_{h,\tau})} \right) \right]^{-1},$$

where $C_{h,\tau}$ is a positive constant which depends from h and τ. By Theorem 4.3.16 we can guarantee that

$$||u_*^\epsilon||_{l_2(\Omega_{h,\tau})} \leq \frac{1}{6C_{h,\tau}} + W_{h,\tau},$$

with $W_{h,\tau} = \sqrt{\frac{1}{36 C_{h,\tau}} - \frac{||f||_{l_2(\Omega_{h,\tau})}}{C_{h,\tau}}}$.

This inequality, together with Theorem 4.3.8, ensures that for sufficiently small h and τ, the following relation

$$1 - C_{h,\tau} \left(||u_*^\epsilon||_{l_2(\Omega_{h,\tau})} + ||u^\epsilon||_{l_2(\Omega_{h,\tau})} \right) > 0$$

holds. Therefore, the convergence of u_* to u depends only on the term $(\mathbf{I})$. Hereby, we have

$$\begin{aligned}
(\mathbf{I}) &= ||T_{h,-\tau}^\epsilon Q_{h,-\tau} T_{h,-\tau}^\epsilon M_{h,\tau}(u^\epsilon) - Q_- T_-^\epsilon M(u^\epsilon)||_{l_2(\Omega_{h,\tau})} \\
&\leq \underbrace{||T_{h,-\tau}^\epsilon Q_{h,-\tau} T_{h,-\tau}^\epsilon \left(M_{h,\tau}^*(u^\epsilon) - M^*(u^\epsilon) \right) ||_{l_2(\Omega_{h,\tau})}}_{(\mathbf{A})} \\
&\quad + \underbrace{||T_{h,-\tau}^\epsilon Q_{h,-\tau} \left(T_{h,-\tau}^\epsilon - T_-^\epsilon \right) M^*(u^\epsilon)||_{l_2(\Omega_{h,\tau})}}_{(\mathbf{B})} + \underbrace{||T_{h,-\tau}^\epsilon \left(Q_{h,-\tau} - Q_+ \right) T_-^\epsilon M^*(u^\epsilon)||_{l_2(\Omega_{h,\tau})}}_{(\mathbf{C})} \\
&\quad + \underbrace{||T_{h,-\tau}^\epsilon Q_{h,-\tau} \left(T_{h,-\tau}^\epsilon - T_-^\epsilon \right) f||_{l_2(\Omega_{h,\tau})}}_{(\mathbf{D})} + \underbrace{||T_{h,-\tau}^\epsilon \left(Q_{h,-\tau} - Q_- \right) T_-^\epsilon f||_{l_2(\Omega_{h,\tau})}}_{(\mathbf{E})},
\end{aligned}$$

where $M^*(u^\epsilon) = |u^\epsilon|^2 u^\epsilon$ and $M_{h,\tau}^*(u^\epsilon)$ denotes its restriction to the space-time grid. By Theorem 4.3.11 we can say that $(\mathbf{B})$ and $(\mathbf{D})$ tend to zero as $h, \tau \to 0$. Also, Theorem 4.3.13

implies the same result for both (**C**) and (**E**). Finally, for (**A**) we have, from the boundedness of the discrete operators, the following relation

$$
\begin{aligned}
&||T^{\epsilon}_{h,-\tau}Q_{h,-\tau}T^{\epsilon}_{h,-\tau}\left(M^{*}_{h,\tau}(u^{\epsilon})-M^{*}(u^{\epsilon})\right)||_{l_2(\Omega_{h,\tau})}\\
&\quad\leq ||T^{\epsilon}_{h,-\tau}Q_{h,-\tau}T^{\epsilon}_{h,-\tau}||_{l_2(\Omega_{h,\tau})}||M^{*}_{h,\tau}(u^{\epsilon})-M^{*}(u^{\epsilon})||_{l_2(\Omega_{h,\tau})}\\
&\quad\leq C_1 C_{h,\tau},
\end{aligned}
$$

where C_1 is a finite constant and $C_{h,\tau}$ is a constant which depends on h and τ and goes to zero with h and τ. Therefore, (**I**) tends to zero when $h,\tau\to 0$, thus, proving our result as $\epsilon\to 0$.

■

To study the rate of convergence of our method for different mesh sizes, we shall present some numerical examples. For simplicity sake, we shall use a cubic space domain $[-a,a]^3$ with an equidistant discretization grid of $(N+1)^3$ points. Also, for the discretization of the time domain we shall consider an equidistant grid with $M+1$ mesh-points.

For all the examples below we will be presenting a table with the l^1-error between the approximated solution and the exact solution at given instants of time.

Example 4.3.18 *As a first example, we consider an exact real-valued c^{∞} solution $u=(0,u_1,u_2,u_3)$ for the Problem (4.12), where*

$$
\begin{aligned}
u_1(x,t) &= e^{-x_1}\ \cos\left(\pi t+\frac{\pi}{2}\right)\ \sin(\pi x_1x_2x_3)\\
u_2(x,t) &= 0\\
u_3(x,t) &= 0,
\end{aligned}
$$

and the corresponding right hand side $f=-\Delta-i\partial_t u-|u^2|u$.

In Table 4.1 we show the approximation error between the exact solution u and its discrete approximation $u_{h,\tau}$ on the domain $\Omega=[-5,5]^3\times[0,2]$ for different mesh sizes.

N	M	t=0	t=0.4	t=0.8	t=1.2	t=1.6	t=2
20	450	2.3313×10^{-3}	1.2799×10^{-3}	5.7386×10^{-4}	2.5728×10^{-4}	1.1633×10^{-4}	5.3040×10^{-5}
25	703	1.5265×10^{-3}	8.3774×10^{-4}	3.7642×10^{-4}	1.6914×10^{-4}	7.5998×10^{-5}	3.4520×10^{-5}
30	1013	1.0765×10^{-3}	5.9073×10^{-4}	2.6569×10^{-4}	1.1950×10^{-4}	5.3548×10^{-5}	2.4266×10^{-5}
35	1378	7.9982×10^{-4}	4.3844×10^{-4}	1.9706×10^{-4}	8.8572×10^{-5}	3.9810×10^{-5}	1.7992×10^{-5}
40	1800	6.1732×10^{-4}	3.3895×10^{-4}	1.5228×10^{-4}	6.8416×10^{-5}	3.0738×10^{-5}	1.3868×10^{-5}
45	2278	4.9075×10^{-4}	2.6919×10^{-4}	1.2107×10^{-4}	5.4362×10^{-5}	2.4450×10^{-5}	1.1014×10^{-5}
50	2813	3.9937×10^{-4}	2.1923×10^{-4}	9.8534×10^{-5}	4.4226×10^{-5}	1.9878×10^{-5}	8.9580×10^{-6}
55	3404	3.3132×10^{-4}	1.8193×10^{-4}	8.1714×10^{-5}	3.6700×10^{-5}	1.6502×10^{-5}	7.4280×10^{-6}

Table 4.1: l_1-error between the approximated solution and the exact solution at different instants.

The following graphics (figures 4.1 and 4.2) show the evolution of the l_1-norm for the approximation error, with respect to the space-mesh and to the time-mesh, respectively.

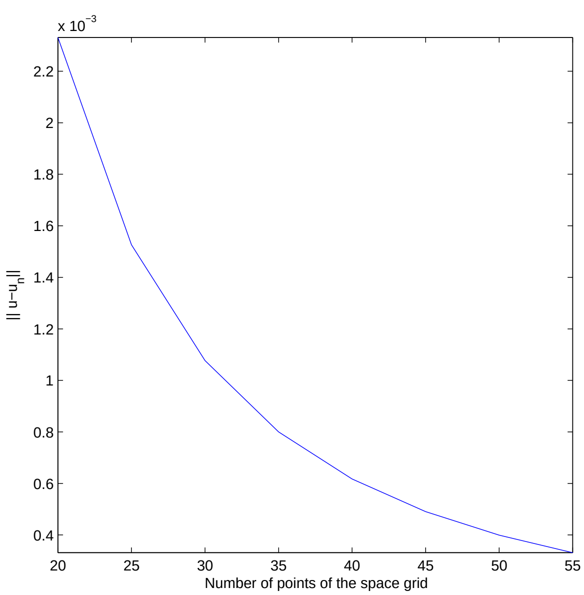

Figure 4.1: l_1-error for different values of N.

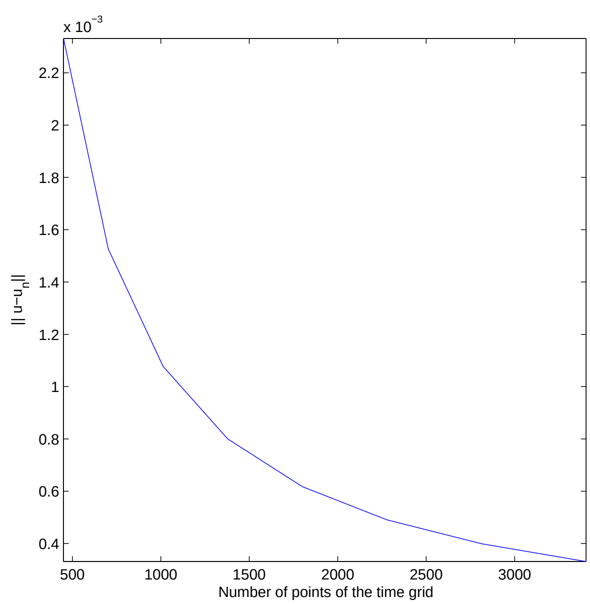

Figure 4.2: l_1-error for different values of M.

Example 4.3.19 *In this example we consider an exact complex-valued C^∞ solution $u = (0, u_1, u_2, u_3)$ of (4.12), where*

$$\begin{aligned} u_1(x,t) &= \left(e^{-t}-1\right)\ (x_1^2-25)\ (x_2^2-25)\ (x_3^2-25) \\ u_2(x,t) &= 0, \\ u_3(x,t) &= \left(e^{-t}-1\right)\ \sin(\pi x_1 x_2 x_3)\ e^{i x_1 t}. \end{aligned}$$

Below is the table with the error of approximation between the exact solution u and its discrete approximation $u_{h,\tau}$ on the domain $\Omega = [-5,5]^3 \times [0,2]$, for different mesh sizes, followed by the graphics (figures 4.3 and 4.4) of the evolution of the approximation error for the correspondent space and time mesh sizes considered.

N	M	t=0	t=0.4	t=0.8	t=1.2	t=1.6	t=2
20	450	4.8846×10^{-3}	2.6819×10^{-3}	1.2024×10^{-3}	5.3907×10^{-4}	2.4374×10^{-4}	1.1140×10^{-5}
25	703	3.1692×10^{-3}	1.7323×10^{-3}	7.8152×10^{-4}	3.5116×10^{-4}	1.5779×10^{-4}	7.1668×10^{-5}
30	1013	2.2183×10^{-3}	1.2172×10^{-3}	5.4746×10^{-4}	2.4623×10^{-4}	1.1033×10^{-4}	5.0000×10^{-5}
35	1378	1.6404×10^{-3}	8.9923×10^{-4}	4.4166×10^{-4}	9.0828×10^{-4}	8.1648×10^{-5}	3.6900×10^{-5}
40	1800	1.2613×10^{-3}	6.9250×10^{-4}	3.1112×10^{-4}	1.8166×10^{-4}	6.2800×10^{-5}	2.8334×10^{-5}
45	2278	9.9988×10^{-4}	5.4847×10^{-4}	2.4668×10^{-4}	1.1076×10^{-4}	4.9816×10^{-5}	2.4428×10^{-5}
50	2813	8.1181×10^{-4}	4.4563×10^{-4}	2.0029×10^{-4}	8.9900×10^{-5}	4.0406×10^{-5}	1.8210×10^{-5}
55	3404	6.7227×10^{-4}	3.6914×10^{-4}	1.6580×10^{-4}	7.4468×10^{-5}	3.3484×10^{-5}	1.5072×10^{-5}

Table 4.2: l_1-error between the approximated solution and the exact solution at different instants.

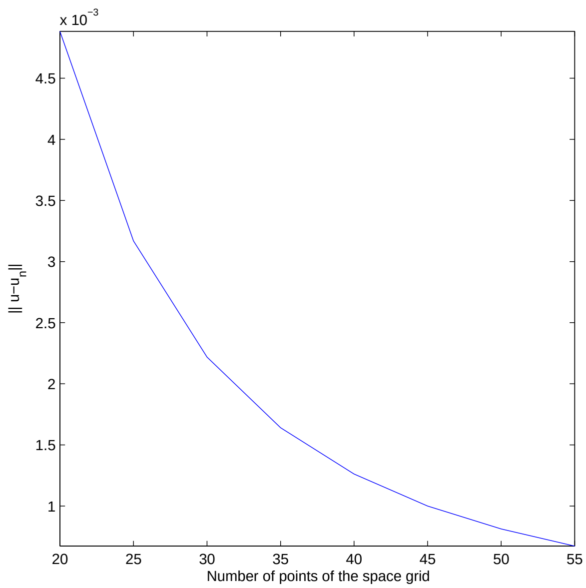

Figure 4.3: l_1-error for different values of N.

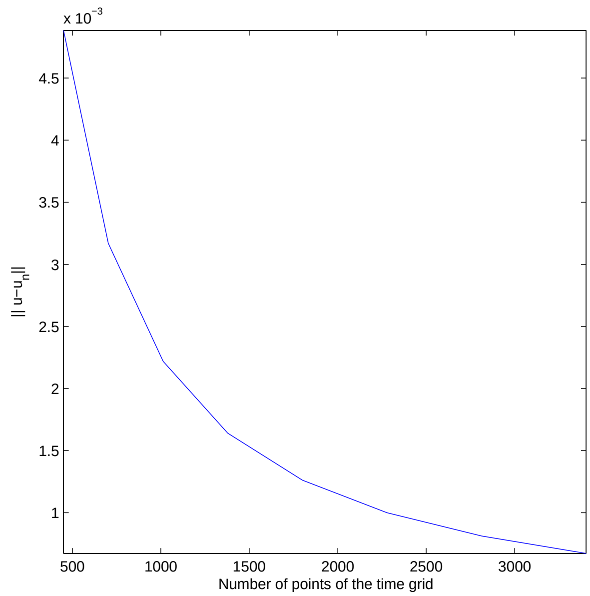

Figure 4.4: l_1-error for different values of M.

Example 4.3.20 *Here we consider an exact solution of lower regularity on the domain* $\Omega = [-5,5]^3 \times [0,2]$, *namely an exact* C^1-*solution* $u = (0, u_1, u_2, u_3)$ *of (4.12), with*

$$\begin{aligned} u_1(x,t) &= (e^{-t}-1)\ (g(x_1)-g(-x_1))\ (g(x_2)-g(-x_2))\ (g(x_3)-g(-x_3)) \\ u_2(x,t) &= 0 \\ u_3(x,t) &= 0, \end{aligned}$$

where g *is the auxiliary B-spline of order 3*

$$g(y) = \begin{cases} \frac{y^3}{6} & \text{if } \ 0 \leq y < 1 \\ -\frac{1}{3} + \frac{y}{2} + \frac{(y-1)^2}{2} - \frac{11(y-1)^3}{24} & \text{if } \ 1 \leq y < 2 \\ \frac{11}{24} + \frac{y}{8} - \frac{7(y-2)^2}{8} + \frac{3(y-2)^3}{8} & \text{if } \ 2 \leq y < 3 \\ \frac{11}{6} - \frac{y}{2} + \frac{(y-3)^2}{4} - \frac{(y-3)^3}{24} & \text{if } \ 3 \leq y \leq 5 \end{cases}.$$

Again, the corresponding right hand side $f = -i\partial_t u - \Delta u - |u^2|u$. *The following table gives the error of approximation between the exact solution* u *and its discrete approximation* $u_{h,\tau}$ *for different mesh sizes considered.*

N	M	t=0	t=0.4	t=0.8	t=1.2	t=1.6	t=2
20	450	5.0846×10^{-3}	2.8819×10^{-3}	1.4024×10^{-3}	7.3907×10^{-4}	2.4437×10^{-4}	1.9111×10^{-4}
25	703	3.7149×10^{-3}	2.0388×10^{-3}	9.1607×10^{-4}	4.1162×10^{-4}	1.8495×10^{-4}	8.4088×10^{-5}
30	1013	2.7242×10^{-3}	1.4948×10^{-3}	6.7232×10^{-4}	3.0239×10^{-4}	1.3550×10^{-4}	6.1402×10^{-5}
35	1378	1.9355×10^{-3}	1.0610×10^{-3}	4.7688×10^{-4}	2.1434×10^{-4}	9.6336×10^{-5}	4.3534×10^{-5}
40	1800	1.4763×10^{-3}	8.1058×10^{-4}	3.6402×10^{-4}	1.6362×10^{-4}	7.3510×10^{-5}	3.3166×10^{-5}
45	2278	1.1856×10^{-3}	6.5030×10^{-4}	2.9248×10^{-4}	1.3133×10^{-4}	5.9066×10^{-5}	2.6610×10^{-5}
50	2813	9.1813×10^{-4}	4.5629×10^{-4}	2.0291×10^{-4}	9.9006×10^{-5}	4.4078×10^{-5}	1.9410×10^{-5}
55	3404	8.0086×10^{-4}	4.3975×10^{-4}	1.9751×10^{-4}	8.8712×10^{-5}	3.9888×10^{-5}	1.7956×10^{-5}

Table 4.3: l_1-error between the approximated solution and the exact solution at different instants.

The next graphics (figures 4.5 and 4.6) show the evolution of the approximation error in l_1-norm for the different space mesh size and time mesh size considered.

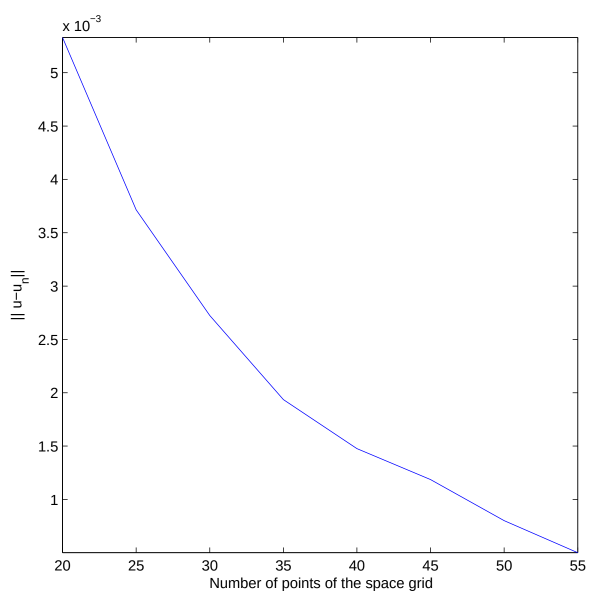

Figure 4.5: l_1-error for different values of N.

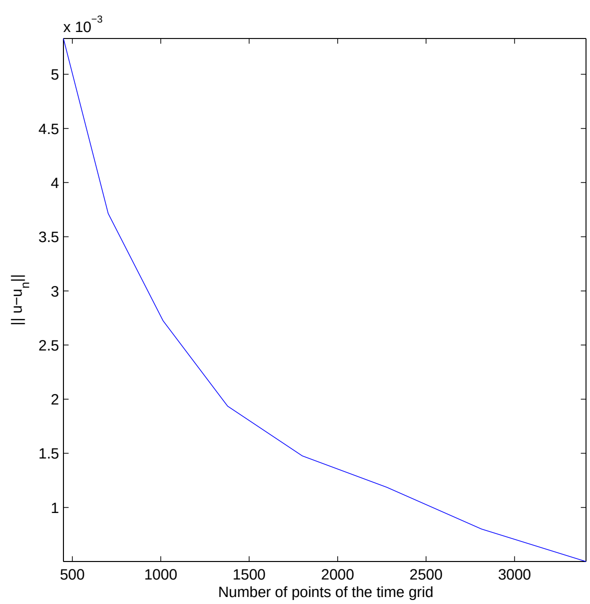

Figure 4.6: l_1-error for different values of M.

Taking into account the previous graphics we are able to observe that the order of convergence for the space coordinate is, in all the examples, of order $\mathcal{O}(h^8)$, while for the time coordinate we get, in all the examples, an order of convergence of order $\mathcal{O}(\tau^{\frac{3}{2}})$. We remark that our method seems to be stable under functions of lower regularity, since the order of convergence for the space and time coordinates remains same in all the three examples.

Conclusion

"The greatest challenge to any thinker is stating the problem in a way that will allow a solution."

Bertrand Russell

In Chapter 2 we showed that the regularized Schrödinger problem can be solved using semigroup and hypoelliptic techniques. As we explained in the beginning of this chapter, in order to control the strong singularity in all the hyperplane $t = 0$ it is necessary to implement a regularization procedure. Hence, we obtain a family of hypoelliptic operators which converge to the original Schrödinger operator, and which can be studied using techniques developed for elliptic operators. The first approach allow us to prove, in a simple way, existence and uniqueness results for solutions of the Schrödinger problem. The same happens when we study a similar problem in the context of non-flat manifolds, where we replace the Laplacian by the Bochner and Günter-Laplacians. Also, we have constructed the parametrix associated to the family of hypoelliptic operators obtained via this regularization procedure. Since our final aim was to make a numerical implementation of the theoretical results, we verified that the obtained results were not satisfactory. The semigroup approach do not provides an explicit expression for our solution while parametrices provide a solution highly dependent on the regularization parameter ϵ, thus carrying instability onto the algorithm.

The third approach, via Clifford algebras, a convenient factorization of the operators and the implementation of an additional regularization procedure proved the most successful for our in so far that it allowed new results about the existence and uniqueness of solutions for several problems involving the Schrödinger operator. The construction of a L_p-decomposition in terms of the kernel of the first order operator D_- allow us to generalize several results valid for the heat operator to the Schrödinger case. However, due to the behavior of the fundamental solution of the second operator, this can only be achieved via the study of the convergence in distributional sense and subsequent study of the limit case in order to ensure strong convergence. Finally, we stress that the arising theory can be implemented numerically with success. In fact, Chapter 4 shown that the results obtained could be constructed in a discrete setting for numerical implementations purposes. An example was given with a (modified version of) cubic NLS equation. From the several results obtained in this Chapter, we point out the convergence of the discrete fundamental solution of the discrete Schrödinger operator to the continuous fundamental solution. This convergence was essential to ensure that all the results obtained in the discrete setting converge, for a fine grid, to the continuous results regarding the resolution of the Schrödinger problem. The numerical examples show that the proposed algorithm has a good order of convergence in both space and time components. Hence, we can say that the algorithm is stable and convergent, even when we are dealing with functions of lower regularity.

This thesis is the starting point for many works, namely the development of a function theory for the family of operators $-\Delta \pm \alpha\partial_t$, with $\alpha \in \mathbb{C}$, using the hypoelliptic approach; application of the algorithm presented in Chapter 4 for non-academic examples,analysis of the behavior of our results in some special domains, for example, the $n-$torus and application of Clifford analysis setting to the analysis of other non-stationary equations from mathematical-physics.

Appendix A

Hypoelliptic Theory

"Like the waves make towards the pebbled shore, so do our minutes hasten to their end"

William Shakespeare, Sonnet 60

In this appendix, we present the definition and necessary properties of hypoelliptic operators, as well as, necessary and sufficient conditions for an operator to be hypoelliptic.

We what follows we use the notations and conventions established on book [4], where we refer the reader for the proofs.

A.1 Definition and main properties

We shall deal with partial differential operators

$$P(D) = \sum_{|p|\leq m} a_p D^p,$$

with $p = (p_1, ..., p_n) \in \mathbb{N}_0^n$, $|p| = p_1 + ... + p_n$, constant coefficients $a_p \in \mathbb{C}$ and $D^p = \dfrac{\partial^{|p|}}{\partial_{x_1}^{p_1} ... \partial_{x_n}^{p_n}}$, such that all distributions solutions of the equation $P(D)u = f$ are always smooth functions whenever f is a smooth function.

Definition A.1.1 *We say that the differential operator $P(D)$ is hypoelliptic if, for every open set $\Omega \subset \mathbb{R}^n$ and every distribution $T \in \mathcal{D}'(\Omega)$, $P(D)T \in C^\infty(\Omega)$ implies $T \in C^\infty(\Omega)$.*

Let $\zeta = (\zeta_1, ..., \zeta_n) \in \mathbb{C}^n$ with $\zeta_j = \xi_j + i\eta_j$, $1 \leq j \leq n$. The polynomial

$$P(\zeta) = \sum_{|p| \leq m} a_p \zeta^p$$

is called the characteristic polynomial (or symbol) of $P(D)$. Denote by $N = \{\zeta \in \mathbb{C}^n : P(\zeta) = 0\}$ the variety of zeros of $P(\zeta)$. For every $\xi \in \mathbb{R}^n$, let

$$d(\xi, N) = \inf_{\zeta \in N} |\xi - \zeta|$$

be the distance from ξ to N.

Theorem A.1.2 *Let $P(\zeta)$ be a constant coefficient polynomial. The following properties are equivalent:*

(H_1) $\zeta \in N$, $|\zeta| \to +\infty$ implies $|\mathrm{Im}\zeta| \to +\infty$;

(H_2) $\xi \in \mathbb{R}^n$, $|\xi| \to +\infty$ implies $d(\xi, N) \to +\infty$;

(H_3) for all $n-$tuples $p = (p_1, ..., p_n)$ with $|p| \neq 0$, $\xi \in \mathbb{R}^n$, $|\xi| \to +\infty$ implies

$$\frac{|P^{(p)}(\xi)|}{|1 + P(\xi)|} \to 0.$$

It can be shown that condition (H_1) is necessary one in order that a differential operator be hypoelliptic. More precisely, we have the following result

Theorem A.1.3 *Let $P(D)$ be a constant coefficient partial differential operator. Suppose that for some open subset $\Omega \subset \mathbb{R}^n$, every $u \in D'(\Omega)$ such that $P(D)u = 0$ belongs to $C^\infty(\Omega)$. Then, property (H_1) holds.*

We observe that if $P(D)$ is hypoelliptic, the hypothesis of Theorem A.1.3 holds, hence $P(D)$ satisfies the condition (H_1) and, by Theorem A.1.2, it satisfies each one of the equivalent conditions (H_1), (H_2) and (H_3). We can state the following result

Theorem A.1.4 *A partial differential operator $P(D)$ is hypoelliptic if and only if in some open subset all distributions solutions of the homogeneous equation $P(D)u = 0$ are C^∞ functions.*

Because of the Theorem A.1.3, we often say that a polynomial $P(\zeta)$ with constant coefficients is hypoelliptic if it satisfies any one of the equivalent conditions (H_1), (H_2) and (H_3). Form now on we shall refer to condition (H) as any one of the conditions (H_1), (H_2) and (H_3).

Condition (H_1) immediately implies that the set of real zeros of P, namely

$$N \cap \mathbb{R}^n = \{\xi \in \mathbb{R}^n : P(\xi) = 0\}$$

is a compact subset of $\mathbb{R}^n$.

Theorem A.1.5 *Let $P(\zeta)$ be a constant coefficient polynomial, let N be its variety of zeros and let d be a real number greater then 1. The following conditions are equivalent*

(dH_1) there is a constant $C > 0$ such that $|\zeta|^{\frac{1}{d}} \leq C(1 + |\mathrm{Im}\zeta|)$, for all $\zeta \in N$;

(dH_2) there is a constant $C' > 0$ such that $|\xi|^{\frac{1}{d}} \leq C'(1 + d(\xi, N))$, for all $\xi \in \mathbb{R}$;

(dH_3) there is a constant $C'' > 0$ such that $|\xi|^{\frac{|p|}{d}} |P^{(d)}(\xi)| \leq C''(1 + |P(\xi)|)$, for all $p \in \mathbb{N}^n$ and all $\xi \in \mathbb{R}^n$.

Condition (dH_2) implies trivially condition (H_2). Conversely, (H_2) implies (dH_2). This is a deeper result whose proof uses the Seidenberg-Tarski excision theorem. More precisely, we have the following result, where (dH) refer to any of the equivalent conditions (dH_1), (dH_2) and (dH_3).

Theorem A.1.6 *Let $P(\zeta)$ be a hypoelliptic polynomial. There is a real number d such that condition (dH) holds. Moreover, the number d for which condition (dH) is valid form a closed half line $[d_0, +\infty[$ with d_0 a rational number greater then 1.*

In summary, conditions (H) and (dH) are all necessary ones, in order that a partial differential operators with constant coefficients be hypoelliptic. In the next section, we will present some sufficient conditions for hypoellipticity.

A.2 Sufficient conditions for hypoellipticity

We start with the definition of fundamental solutions and parametrices of a partial differential operator with constant coefficients in $\mathbb{R}^n$.

Definition A.2.1 *We say that a distribution E is a fundamental solution of the operator $P(D)$ if $P(D)E = \delta$, where δ denotes the Dirac measure.*

The above formula means that, for every test function $\phi \in C^\infty(\mathbb{R}^n)$, $< P(D)E, \phi >=< E, P(D)^t \phi >= \phi(0)$. Here, $P(D)^t$ denotes the transpose of $P(D)$ defined by

$$P(D)^t = \sum_p (-1)^{|p|} a_p D^p.$$

Notice that we can also write $P(D)^t = P(-D)$.

Definition A.2.2 *A distribution $E \in D'(\mathbb{R}^n)$ is said to be a parametrix of $P(D)$ if the distribution $R = P(D) - \delta$ is a integrable function in some open neighborhood of the origin in $\mathbb{R}^n$. The distribution R is called the rest of the parametrix.*

Hypoelliptic operators can be characterized in terms of regularity properties of their fundamental solutions. We have the following result.

Theorem A.2.3 *Let $P(D)$ be a partial differential operator with constants coefficients. If $P(D)$ is hypoelliptic then every fundamental solution is C^∞ in $\mathbb{R}^n \setminus \{0\}$. Conversely, if there is a fundamental solution which is a C^∞ function in $\mathbb{R}^n \setminus \{0\}$ then $P(D)$ is hypoelliptic.*

A well know theorem proved by Malgrange [50] and Ehrenpreis [26] states that every partial differential operator with constant coefficients possesses a fundamental solution. This result combined with Theorem A.2.3 imply that, in order to show that an operator $P(D)$ is hypoelliptic, it suffices to show that it has at least one fundamental solution which is C^∞ in $\mathbb{R}^n \setminus \{0\}$. When this is the case, all fundamental solutions will be C^∞ in $\mathbb{R}^n \setminus \{0\}$.

In view of Theorem A.2.3, in order to prove that a partial differential operator $P(D)$ is hypoelliptic, it suffices to construct a fundamental solution which is C^∞ in $\mathbb{R}^n \setminus \{0\}$. Actually, it suffices to construct a parametrix with smooth rest.

Theorem A.2.4 *If a differential operator $P(D)$, with constant coefficients, has a parametrix which is a C^∞ function in $\mathbb{R}^n \setminus \{0\}$ and a rest which is a C^∞ function in $\mathbb{R}^n$, then $P(D)$ is hypoelliptic.*

Bibliography

[1] Artino, R., Gevrey classes and hypoelliptic boundary-value problems, *Pac. J. of Math.*, **63** No.1, (1976), 1-21. {−}

[2] Artino, R., On semielliptic boundary-value problems, *J. Math. Anal. Appl.*, **42** No.3, (1973), 610-626. {−}

[3] Artino, R.A. and Barros-Neto, J., Matrix Triangulation of Hypoelliptic Boundary Value Problems, *Annales de l'Institut Fourier, Grenoble* **42(4)**, (1992), 805-824. {29,31}

[4] Artino R and Barros-Neto J. *Hypoelliptic Boundary-Value Problems.* Lectures Notes in Pure and Applied Mathematics - Vol 53. Marcel Dekker, 1980. {34,35,115}

[5] Barros-Neto, J., On regular hypoelliptic boundary-value problems, *J. Math. Anal. Appl.*, **41** No.2, (1973), 508-530. {−}

[6] Barros-Neto, J., The parametrix of a regular hypoelliptic boundary-value problem. *Ann. Sc. Norm. Suop. Pisa.*, **26** No.1, (1972), 247-254. {*ix*}

[7] Bergamasco, A.P. and Petronilho, G., A construction of parametrices of elliptic boundary value problems, *Portugalie Mathematica*, **50**(3), (1993), 263-276. {28}

[8] Berline, N., Getzler, E. and Vergne, M., Heat Kernel and Dirac operators, *Grundlehren der Mathematischen Wissenschaften,* **198**, Springer-Verleng, London, 1992. {−}

[9] Bernstein, S., Factorization of the nonlinear Schrödinger equation and applications, *Compp. Var. and Ellipp. Eq. - special issue: a tribute to R. Delanghe*, **51** No.5-6, (2006), 429-452. {78}

[10] Boor, C. and Höllig, K., Fundamental solutions for multivariate difference equations, *Am. J. Math.*, **111** No.3, (1989), 403-415. {−}

[11] Brackx F., Delanghe R. and Sommen F. *Clifford Analysis*. Research Notes in Mathematics **76**. Pitman: London, 1982. {1}

[12] Brink, L. and Schwartz, J.H., Quantum superspace, *Phy. Lett.*, **B100**, (1981), 310-312. {*viii*}

[13] Cerejeiras, P. and Vieira, N., On the fundamental solutions of the Schrödinger operator, accepted for publication in *Journal of Difference Equations and Applications.* {72}

[14] Cerejeiras, P. and Vieira, N., Regularization of the Non Stationary Schrödinger Operator, *Math. Meth. in Appl. Sc.*, **32** No.4, (2009), 535-555. {87}

[15] Cerejeiras, P., Faustino, N. and Vieira, N., Numerical Clifford analysis for the nonlinear Schrödinger problem, *Numer. Methods Partial Differ. Equations*, **24** No.4, (2008), 1181-1202. {72}

[16] Cerejeiras, P., Sommen, F. and Vieira, N. , Fischer decomposition and special solutions for the parabolic Dirac operator, *Math. Meth. in Appl. Sc.*, **18**, (2008), 1023-1032. {−}

[17] Cerejeiras, P. and Vieira, N., Factorization of the nonstationary Schrödinger operator, *Adv. Appl. Clifford Algebr.*, **17**, (2007), 331-341. {27,35,47,65,78,104}

[18] Cerejeiras, P., Faustino, N. and Vieira, N., Numerical clifford analysis for nonlinear time-dependent problems, **in:** Proceedings of CMMSE 2006, Vol I, (2006), 196-203. {72}

[19] Cerejeiras, P., Kähler, U. and Sommen F., Parabolic Dirac operators and the Navier-Stokes equations over time-varying domains, *Math. Meth. in Appl. Sc.*, **28**, (2005), 1715-1724. {*viii*,38,61}

[20] Clifford, W.K., On the classification of geometric algebras, **in:** Tucker, R. (ed.), *Mathematical Papers*, Macmillian, London, 1882, 397-401. {−}

[21] Cnops, J., *An introduction to Dirac operators on Manifolds*, Birkhäuser, 2002. {−}

[22] Delanghe, R., Sommen, F. and Souček, *Clifford algebras and spinor-valued functions,* Kluwer Academic Publishers, 1992. {1,20,40,41}

[23] Dirac, P.A.M., The quantum theory of the electron, *Proc. Roy. Soc. London*, **A117**, (1928), 610-624. {*viii*}

[24] Dixon, G., Algebraic Unification, *Phy. Rev.*, **D28**, (1983), 833-843. {*viii*}

[25] Duduchava, L.R., Mitrea, D. and Mitrea, M., *Differential operators and boundary value problems on hypersurfaces*, Math. Nachr., **279** No.9-10, (2006), 996-1023. {13,14}

[26] Ehrenpresis, L., Solution of some problems of division, *I. Am. J. Math.*, **76**, (1954), 883-903. {118}

[27] Estrada, R., Regularization of distributions, *Inter. J. Math. and Math. Sci.*, **21** No.4, (1998), 625-636. {−}

[28] Eichhorn, J. (1991). The heat semi-group acting on tensors or differential forms with values in vector bundle. *Arch. Math.* 27(1):15-24. {*ix*,18,20,21}

[29] Evans, L.C., *Partial Differential Equations*, American Mathematical Society, 1991. {20,26}

[30] Faustino, N. and Vieira, N., Numerical Clifford analysis for the non-stationary Schrödinger equation, **in:** *Proceedings of ICNAAM 2007*, T. Simos et al (eds.), AIP Conference Proceedings, (2007), 742-745. {72}

[31] Faustino, N., Gürlebeck, K., Hommel, A. and Kähler, Difference potentials for the Navier-Stokes equations in unbounded domains, *J. Difference Equ. Appl.*, **12** No.6, (2006), 577-595. {72}

[32] Fournier, J.F. and Adams, R.A., *Sobolev Spaces*, Academic Press, 2003. {−}

[33] Habala, P., Hájek, P. and Zizler, V., *Introduction to Banach Spaces I*, Matfyzpress, Vydavatelství Matematicko-fyzikální fakulty Univerzity Karlovy, 1996. {18}

[34] Gilbert, J.E. and Murray, M., *Clifford algebras and Dirac operators in harmonic analysis*, Cambridge studies in advanced mathematics **26**, Cambridge University Press, 1991. {1,13}

[35] Graaf, J., *Evolution Equations*, Textos de Matemática - Série B - No.14, Departamento de Matemática - Faculdade de Ciências e Tecnologia da Universidade de Coimbra, 1998. {−}

[36] Günter, N., *Potential theory and its application to the basic problems of mathematical physics*, Fizmatgiz, 1953 (Russian translation in French: Gauthier-Villars, Paris, 1994). {14}

[37] Gürlebeck, K. and Hommel, A., On finite difference Dirac operators and their fundamental solutions, *Adv. Appl. Clifford Algebr.*, **11**, (2001), 89-106. {*x*,72,80,81}

[38] Gürlebeck, K. and Hommel, A., On fundamental solutions of the heat conduction difference operator, *ZAA*, **11** No.3, (1994), 1-16. {72,79,82,93}

[39] Gürlebeck, K. and Sprößig, W., *Quaternionic and Clifford calculus for physicists and engineers*, John Wiley and Sons, 1997. {1,6,7,8,37,57,60,71,72,79,81,101}

[40] Hestenes, D., *Spacetime algebra*, Gordon and Breach, 1966. {*viii*}

[41] Hommel, A., Fundamentallösungen partieller Differentialoperatoren und die Lösung diskreter Randwertprobleme mit Hilfe von Differenzenpotentialen, PhD tesis, Bauhaus-Universität Weimar, Germany, 1998. {82,84}

[42] Hörmander, L., *The Analysis of Linear Partial Differential Operators III: Pseudo-Differential Operators*, A Series of Comprehensive Studies in Matehmatics - 274, Springer-Verlang, 1984. {27,40}

[43] Hörmander, L., On the regularity of the solutions of boundary problems, *Acta Matematica*, **99**, (1958), 225-264. {*ix*}

[44] Hoskins, R.F. and Pinto, J.S., *Theories of Generalised Functions Distributions, Ultradistributions and Other Generalised Functions,* Horwood, 2005. {49}

[45] Imaeda, K., A new formulation of classical electrodynamics, *Nuovo Cim.*, **B32**, (1976), 138-159. {*viii*}

[46] Kravchenko, V.G. and Kravchenko, V.V., Quaternionic factorization of the Schrödinger operator and its applications to some first-order systems of mathematical physics, *J. Phys. A: Math. Gen.*, **36** No.44, (2000), 11285-11297. {−}

[47] Kravchenko, V.G. and Shapiro, M.V., *Integral representations for spatial models of mathematical physics*, Pitman Research Notes in Math., Series 351, 1996. {37}

[48] Lee, J.M., *Riemannian Manifolds: An Introduction to Curvature*, Springer, 1997. {10}

[49] Leutwiler, H. (1996). Remarks on modified Clifford analysis. *Potential theory - ICPT'94. Proceedings of the international conference, Kouty, Czech Republic, August 13-20*, Berlin: deGruyter, Král, J. (ed.), 389-397. {13}

[50] Malgrange, B., Existence et approximation des solutions des equations aux derivees partielles et des equations de convolution, *Ann. Inst. Fourier.* **6**, (1955-56), 271-355. {118}

[51] Mikhlin, S.G. and Prössdorf, S., *Singular Integral Operators*, Springer-Verlag, 1986. {51,52}

[52] Olver, Peter J., *Applications of Lie Groups to Differential Equations*, Graduated Texts in Mathematics, **107**, 2nd Ed., Springer-Verlag, 1993. {13}

[53] Onsager, L., Crystal Statistics I: a two-dimensional model with an order-disorder transition, *Phys. Rev.*, **65**, (1944), 117-149. {*viii*}

[54] Park, E., *Complex Topological K-Theory*, Cambridge studies in advanced mathematics **111**, Cambridge University Press, 2008. {−}

[55] Reed, M. and Simon, B., *Methods of modern mathematical physics, II, Fourier analysis, self-adjointness*, New York, Academic Press, 1975. {19}

[56] Riesz, M., *Clifford numbers and spinors - Lecture Notes No.38*, Institut for Fluid Dynamics and Applied Mathematics, University of Maryland, College Park, 1958. {*viii*}

[57] Ryabenkij, V.S., *The method of difference potentials for some for some problems of continuum mechanics*, Nauka, Moskva, 1987 (russian). {72}

[58] Schrödinger, E., An undulatory theory of the Mechanics of atoms and molecules, *Phy. Rev.*, **28** No.6, (1926), 1049-1070. {−}

[59] Salingaros, N., Electromagnetism and the holomorphic properties of spacetime, *J. Math. Phys.*, **22**, (1981), 1919-1925. {*viii*}

[60] Shapiro, M. and Kravchenko, V.V., *Integral representation for spatial models of mathematical physics*, Pitman research notes in mathematics series **351**, Harlow, Longman, 1996. {−}

[61] Stern, I., Boundary value problems for generalized Cauchy-Riemann systems in the space, **in:** Kühnau, R. and Tutschke, W. (ed.), *Boundary value and initial value problems in complex analysis*, Pitman Res. Notes in Math., **256**, (1991), 159-183. {82,84}

[62] Stummel, F., Elliptische Differenzenoperatoren unter Dirichlet-Randbedingungen, *Math. Zeitschrift*, **97**, (1967), 169-211. {82}

[63] Sullivan, D.M., Determining a complete three-dimensional set of eigenfunctions for nanoscale structure analysis, *J. Appl. Phys.*, **98**, (2005), 084311- {71}

[64] Tao, T., *Nonlinear Dispersive Equations, Local and Global Analysis,* CBMS Regional Conference Series in Mathematics, vol 106, American Mathematical Society: Providence, RI, 2006. {*viii*,16,17,46}

[65] Triebel, H. *Interpolation Theory, Function spaces, differential operators,* VEB Deutscher Verlag der Wissenschaften, Berlin, 1978. {6}

[66] Velo, G., Mathematical Aspects of the nonlinear Schrödinger Equation, **in:** Vásquez, Luis et al. (ed.), *Proceedings of the Euroconference on nonlinear Klein-Gordon and Schrödinger systems: theory and applications*, Singapore: World Scientific, 1996, 39-67. {*viii*,27,61,66,69}

[67] Vieira, N., Powers of the parabolic Dirac operator, *Adv. Appl. Clifford Algebr.*, **18**, (2008), 1023-1032. {−}

[68] Voigt, J., Absorption semigroups, their generators, and Schrödinger semigroups, *J. Func. Anal.*, **67**, (1986), 167-205. {18}

[69] Yosida, K., *Functional Analysis*, A Series of Comprehensive Studies in Mathematics - 123, Springer-Verlag, Berlin Heidelberg New York, 1978. {18,19}

[70] Zhao, Z., *From Brownian motion to Schrödinger Equation*, Springer-Verlag, 1995. {*ix*,20}

Index